

Robust dimension-free Gram operator estimates

Ilaria Giulini*

INRIA Saclay

e-mail: ilaria.giulini@me.com

Abstract: In this paper we investigate the question of estimating the Gram operator by a robust estimator from an i.i.d. sample in a separable Hilbert space and we present uniform bounds that hold under weak moment assumptions. The approach consists in first obtaining non-asymptotic dimension-free bounds in finite-dimensional spaces using some PAC-Bayesian inequalities related to Gaussian perturbations of the parameter and then in generalizing the results in a separable Hilbert space. We show both from a theoretical point of view and with the help of some simulations that such a robust estimator improves the behavior of the classical empirical one in the case of heavy tail data distributions.

MSC 2010 subject classifications: 62G35, 62G05.

Keywords and phrases: PAC-Bayesian learning, Gram operator, dimension-free bounds, robust estimation.

1. Introduction

Many algorithms, such as spectral clustering, kernel principal component analysis or more generally kernel-based methods, are based on estimating eigenvalues and eigenvectors of integral operators defined by a kernel function, from a given random sample. To set the context from a statistical point of view, let $\mu \in \mathcal{M}_+^1(\mathcal{X})$ be an unknown probability distribution on a compact space \mathcal{X} and let k be a kernel on \mathcal{X} . The goal is to estimate the integral operator

$$L_k f(x) = \int k(x, z) f(z) d\mu(z)$$

from an i.i.d. random sample drawn according to μ .

A first study on the relationship between the spectral properties of a kernel matrix and the corresponding integral operator can be found in [Koltchinskii, V. and Giné, E. \(2000\)](#) for the case of a symmetric square integrable kernel k . They prove that the ordered spectrum of the kernel matrix $K_{ij} = \frac{1}{n}k(X_i, X_j)$ converges to the ordered spectrum of the kernel integral operator L_k . Connections between this empirical matrix and its continuous counterpart have been subject

*The results presented in this paper were obtained while the author was preparing her PhD under the supervision of Olivier Catoni at the Département de Mathématiques et Applications, École Normale Supérieure, Paris, with the financial support of the Région Île de France.

of much research, for example in the framework of kernel-PCA (e.g. Shawe-Taylor, J., Williams, C. and Cristianini, C. and Kandola, J. (2005), Shawe-Taylor, J., Williams, C. and Cristianini, C. and Kandola, J. (2005), Zwald, L., Bousquet, O. and Blanchard, G. (2004)) and spectral clustering (e.g. von Luxburg, U., Belkin, M. and Bousquet, O. (2008)). In Rosasco, L., Belkin, M. and De Vito, E. (2010), the authors study the connection between the spectral properties of the empirical kernel matrix K_{ij} and those of the corresponding integral operator L_k by introducing two extension operators on the (same) reproducing kernel Hilbert space defined by k , that have the same spectrum (and related eigenfunctions) as K and L_k respectively. In such a way they overcome the difficulty of dealing with objects (K and L_k) operating in different spaces. The integral operator L_k is related to the Gram operator

$$\mathcal{G}v = \int \langle v, \phi(z) \rangle_{\mathcal{K}} \phi(z) \, d\mu(z), \quad v \in \mathcal{K},$$

where \mathcal{K} denotes the reproducing kernel Hilbert space defined by the kernel k and ϕ the corresponding feature map.

The main objective of this paper is to estimate Gram operators on (infinite-dimensional) Hilbert spaces. Some bounds on the deviation of the empirical Gram operator from the true Gram operator in separable Hilbert spaces can be found in Koltchinskii, V. and Lounici, K. (2014) in the case of Gaussian random vectors.

Let us introduce some notation. We denote by \mathcal{H} a separable Hilbert space and by $P \in \mathcal{M}_+^1(\mathcal{H})$ a (possibly unknown) probability distribution on \mathcal{H} . Remark that with the above notation $P = \mu \circ \phi^{-1}$. Our goal is to estimate the Gram operator $\mathcal{G} : \mathcal{H} \rightarrow \mathcal{H}$ defined as

$$\mathcal{G}v = \int \langle v, z \rangle_{\mathcal{H}} z \, dP(z)$$

from an i.i.d. sample drawn according to P . Our approach consists in first considering the finite-dimensional setting where X is a random vector in \mathbb{R}^d and then in generalizing the results to the infinite-dimensional case of separable Hilbert spaces. To be able to go from finite to infinite dimension we will establish dimension-free inequalities. To be more precise, we consider the related problem of estimating the quadratic form

$$N(\theta) = \langle \mathcal{G}\theta, \theta \rangle_{\mathcal{H}}, \quad \theta \in \mathcal{H}$$

which rewrites explicitly as

$$N(\theta) = \int \langle \theta, z \rangle_{\mathcal{H}}^2 \, dP(z).$$

In the finite-dimensional setting we construct an estimator of the quadratic form $N(\theta)$ and we provide non-asymptotic dimension-free bounds for the approximation error that hold under weak moment assumptions. Observe that in

the finite-dimensional case the quadratic form $N(\theta)$ can be seen as the quadratic form associated to the Gram matrix

$$G = \int xx^\top dP(x).$$

Observe also that the study of the Gram matrix is of interest in the case of a non-centered criterion and it coincides, in the case of centered data (i.e. $\mathbb{E}[X] = 0$), with the study of the covariance matrix

$$\Sigma = \mathbb{E} [(X - \mathbb{E}[X])(X - \mathbb{E}[X])^\top].$$

Many theoretical results have been proposed on the estimation of covariance matrices, e.g. [Rudelson, M. \(1999\)](#), [Vershynin, R. \(2012\)](#), [Tropp, J. A. \(2012\)](#). These results follow from the study of random matrix theory and use as an estimator of G the matrix obtained by replacing the unknown probability distribution P with the sample distribution $\frac{1}{n} \sum_{i=1}^n \delta_{X_i}$. In [Rudelson, M. \(1999\)](#) the non-commutative Khintchine inequality is used to obtain bounds on the sample covariance matrix of a bounded random vector. Non-asymptotic results are obtained in [Vershynin, R. \(2012\)](#) as a consequence of the analysis of random matrices with independent rows, while in [Tropp, J. A. \(2012\)](#) the author uses an extension of the Bernstein inequality to matrices. However, such an empirical estimator becomes less efficient when the data have a long tail distribution. In [Minsker, S.](#) the author presents a different estimator based on the geometrical median which is more robust than the classical empirical one.

We first present a way to construct a robust estimator of the Gram matrix G in finite dimension and then we extend the results to the infinite-dimensional case.

The paper is organized as follows. Section 2 deals with the finite-dimensional case. We provide a new robust estimator of the Gram matrix G and we use a PAC-Bayesian approach to obtain non-asymptotic dimension-independent bounds of its approximation error. In section 3 we extend the results to the infinite-dimensional case, taking advantage of the fact that they are independent of the dimension of the ambient space. In section 4 we propose some empirical results to show the performance of our estimator. In Appendix A we compare from a theoretical point of view the behavior of our robust estimator to the one of the classical empirical estimator. Finally in Appendix B we extend the results to estimate the expectation of a symmetric random matrix and we consider the problem of estimating the covariance matrix in the case when the expectation is unknown.

2. The finite-dimensional setting

Let $P \in \mathcal{M}_+^1(\mathbb{R}^d)$ be an unknown probability distribution on \mathbb{R}^d and let $X \in \mathbb{R}^d$ be a random vector of law P . We denote by \mathbb{E} the expectation with respect to

P. Our goal is to estimate the quadratic form

$$N(\theta) = \mathbb{E}[\langle \theta, X \rangle^2], \quad \theta \in \mathbb{R}^d,$$

(that computes the energy in the direction θ) from an i.i.d. sample $X_1, \dots, X_n \in \mathbb{R}^d$ drawn according to P. Observe that $N(\theta)$ can be seen as the quadratic form associated to the Gram matrix

$$G = \mathbb{E}[XX^\top].$$

Indeed to recover the Gram matrix G from the above quadratic form it is sufficient to use the polarization identity

$$\begin{aligned} G_{ij} &= e_i^\top G e_j = \frac{1}{4} [(e_i + e_j)^\top G (e_i + e_j) - (e_i - e_j)^\top G (e_i - e_j)] \\ &= \frac{1}{4} [N(e_i + e_j) - N(e_i - e_j)] \end{aligned}$$

where $\{e_i\}_{i=1}^d$ is the canonical basis of \mathbb{R}^d .

A classical empirical estimator of the quadratic form $N(\theta)$ is

$$\bar{N}(\theta) = \frac{1}{n} \sum_{i=1}^n \langle \theta, X_i \rangle^2$$

obtained by replacing the unknown probability distribution P with the sample distribution. However, as shown in [Catoni, O. \(2012\)](#), if the distribution of $\langle \theta, X \rangle^2$ has a heavy tail for some values of θ , the quality of the approximation provided by the classical empirical estimator can be improved, using some M -estimator with a suitable influence function and a scale parameter depending on the sample size. Thus, for any $\theta \in \mathbb{R}^d$ and any $\lambda > 0$, we consider

$$r_\lambda(\theta) = \frac{1}{n} \sum_{i=1}^n \psi(\langle \theta, X_i \rangle^2 - \lambda), \quad (2.1)$$

where the function $\psi : \mathbb{R} \rightarrow \mathbb{R}$, defined as

$$\psi(t) = \begin{cases} \log(2) & \text{if } t \geq 1 \\ -\log\left(1 - t + \frac{t^2}{2}\right) & \text{if } 0 \leq t \leq 1 \\ -\psi(-t) & \text{if } t \leq 0 \end{cases} \quad (2.2)$$

is symmetric non-decreasing and bounded and satisfies

$$-\log\left(1 - t + \frac{t^2}{2}\right) \leq \psi(t) \leq \log\left(1 + t + \frac{t^2}{2}\right), \quad t \in \mathbb{R}.$$

Introduce

$$\hat{\alpha}(\theta) = \sup\{\alpha \in \mathbb{R}_+ \mid r_\lambda(\alpha\theta) \leq 0\} \quad (2.3)$$

and observe that, since the function $\alpha \mapsto r_\lambda(\alpha\theta)$ is continuous, $r_\lambda(\hat{\alpha}(\theta)\theta) = 0$ as soon as $\hat{\alpha}(\theta) < +\infty$. Moreover, since the function ψ is close to the identity in a neighborhood of the origin,

$$0 = r_\lambda(\hat{\alpha}(\theta)\theta) \simeq \hat{\alpha}(\theta)^2 \bar{N}(\theta) - \lambda$$

and therefore it is natural to consider as an estimator of $N(\theta)$ a quantity related to $\lambda/\hat{\alpha}(\theta)^2$, for a suitable value of λ . We consider the family of (robust) estimators

$$\tilde{N}_\lambda(\theta) = \frac{\lambda}{\hat{\alpha}(\theta)^2} \quad (2.4)$$

and we observe that, since $\hat{\alpha}(\theta)$ is homogeneous of degree -1 in θ ,

$$\tilde{N}_\lambda(\theta) = \|\theta\|^2 \tilde{N}_\lambda(\theta/\|\theta\|).$$

In the following we will use a PAC-Bayesian approach linked to Gaussian perturbations of the parameter θ to first construct a confidence region for $N(\theta)$ and then define and study a robust estimator by choosing a suitable value $\hat{\lambda}$ for the parameter λ .

Given $\theta \in \mathbb{R}^d$, we consider the family of Gaussian perturbation $\pi_\theta \sim \mathcal{N}(\theta, \beta^{-1}\mathbf{I})$ of mean the true value θ and covariance matrix $\beta^{-1}\mathbf{I}$ where $\beta > 0$ is a free parameter.

Let $\Lambda \subset (\mathbb{R}_+ \setminus \{0\})^2$ be a finite set of possible values of the couple of parameters (λ, β) and $|\Lambda|$ its cardinality. Let us introduce

$$s_4 = \mathbb{E}[\|X\|^4]^{1/4} \quad \text{and} \quad \kappa = \sup_{\substack{\theta \in \mathbb{R}^d \\ \mathbb{E}[\langle \theta, X \rangle^2] > 0}} \frac{\mathbb{E}[\langle \theta, X \rangle^4]}{\mathbb{E}[\langle \theta, X \rangle^2]^2} \quad (2.5)$$

assuming that these two quantities are finite.¹ For any $(\lambda, \beta) \in \Lambda$ and $\epsilon > 0$, we put

$$\begin{aligned} \xi &= \frac{\kappa\lambda}{2}, \\ \mu &= \lambda(\kappa - 1) + \frac{(2+c)\kappa^{1/2}s_4^2}{\beta}, \\ \gamma &= \frac{\lambda}{2}(\kappa - 1) + \frac{(2+c)\kappa^{1/2}s_4^2}{\beta} + \frac{(2+3c)s_4^4}{2\beta^2\lambda} + \frac{\log(|\Lambda|/\epsilon)}{n\lambda}, \\ \delta &= \frac{\beta}{2n\lambda}, \end{aligned} \quad (2.6)$$

where

$$c = \frac{15}{8\log(2)(\sqrt{2}-1)} \exp\left(\frac{1+2\sqrt{2}}{2}\right) \leq 44.3. \quad (2.7)$$

¹As it will be explained later, it is sufficient to know an upper bound for these quantities since the following results still hold true replacing s_4 and κ by their upper bounds.

Proposition 2.1. *With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$, any $(\lambda, \beta) \in \Lambda$,*

$$\Phi_{\theta,-}\left(\frac{\lambda}{\widehat{\alpha}(\theta)^2}\right) \leq N(\theta) \leq \Phi_{\theta,+}^{-1}\left(\frac{\lambda}{\widehat{\alpha}(\theta)^2}\right)$$

where $\Phi_{\theta,-}$ and $\Phi_{\theta,+}$ are non-increasing functions defined as

$$\begin{aligned} \Phi_{\theta,-}(t) &= t \left(1 - \frac{\gamma + \delta\lambda\|\theta\|^2/t}{1 + \mu - \gamma - \delta\lambda\|\theta\|^2/t} \right) \mathbb{1} \left[\xi - \mu + 2\gamma + 2\delta\lambda\|\theta\|^2/t < 1 \right] \\ \Phi_{\theta,+}(t) &= t \left(1 + \frac{\gamma + \delta\lambda\|\theta\|^2/t}{1 - \mu - \gamma - 2\delta\lambda\|\theta\|^2/t} \right)^{-1} \mathbb{1} \left[\xi + \mu + \gamma + 2\delta\lambda\|\theta\|^2/t < 1 \right]. \end{aligned}$$

For the proof we refer to section 5.1.

Observe that since those functions depend on θ only through $\|\theta\|$, if θ is such that $\|\theta\| = 1$ it is natural to omit the dependence of θ and write Φ_- and Φ_+ . In the following we will omit the dependence of θ of the functions defined in Proposition 2.1, so that we write Φ_- and Φ_+ instead of $\Phi_{\theta,-}$ and $\Phi_{\theta,+}$.

Proposition 2.2. *Let $\sigma \in \mathbb{R}_+$ be any energy level. We consider the set*

$$\Gamma = \left\{ (\lambda, \beta, t) \in \Lambda \times \mathbb{R}_+ \mid \xi + \mu + \gamma + 2\frac{\delta\lambda}{\max\{t, \sigma\}} < 1 \right\}$$

and the bound

$$B_{\lambda,\beta}(t) = \begin{cases} \frac{\gamma + \lambda\delta/\max\{t, \sigma\}}{1 - \mu - \gamma - 2\lambda\delta/\max\{t, \sigma\}} & (\lambda, \beta, t) \in \Gamma \\ +\infty & \text{otherwise.} \end{cases} \quad (2.8)$$

With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$, any $(\lambda, \beta) \in \Lambda$,

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\widetilde{N}_\lambda(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq B_{\lambda,\beta} \left[\|\theta\|^{-2} \widetilde{N}_\lambda(\theta) \right].$$

Proof. We observe that, for any $z, t, \sigma \in \mathbb{R}_+$, if $\Phi_+(z) \leq t$ then

$$\Phi_+(\max\{z, \sigma\}) \leq \max\{t, \sigma\}$$

since, by definition $\Phi_+(\sigma) \leq \sigma$ and similarly if $\Phi_-(z) \leq t$, then

$$\Phi_-(\max\{z, \sigma\}) \leq \max\{t, \sigma\}.$$

Thus, according to the definition of $B_{\lambda,\beta}$ in equation (2.8), we get

$$\Phi_+(\max\{z, \sigma\}) = \max\{z, \sigma\} \left(1 + B_{\lambda,\beta}(z) \right)^{-1} \quad (2.9)$$

$$\Phi_-(\max\{z, \sigma\}) \geq \max\{z, \sigma\} \left(1 - B_{\lambda,\beta}(z) \right) \quad (2.10)$$

and moreover

$$\Phi_+^{-1}(\max\{z, \sigma\}) \leq \max\{z, \sigma\} \left(1 + B_{\lambda, \beta}(z)\right)$$

which concludes the proof. \square

From now on we fix the finite set Λ of all possible values of the couple (λ, β) as

$$\Lambda = \{(\lambda_j, \beta_j) \mid 0 \leq j < K\}, \quad (2.11)$$

where $K = 1 + \left\lceil a^{-1} \log \left(\frac{n}{72(2+c)\kappa^{1/2}} \right) \right\rceil$, with $a > 0$, and

$$\begin{aligned} \lambda_j &= \sqrt{\frac{2}{n(\kappa-1)} \left(\frac{(2+3c)}{4(2+c)\kappa^{1/2} \exp(-ja)} + \log(K/\epsilon) \right)} \\ \beta_j &= \sqrt{2(2+c)\kappa^{1/2}s_4^4 n \exp[-(j-1/2)a]}. \end{aligned}$$

We put

$$(\hat{\lambda}, \hat{\beta}) = \arg \min_{(\lambda, \beta) \in \Lambda} B_{\lambda, \beta} \left[\|\theta\|^{-2} \tilde{N}_\lambda(\theta) \right]$$

and we define our robust estimator as

$$\hat{N}(\theta) = \tilde{N}_{\hat{\lambda}}(\theta). \quad (2.12)$$

Proposition 2.3. *Let us fix a threshold $\sigma \leq s_4^2$ and set the value of the parameter a to $1/2$. Introduce*

$$\zeta_*(t) = \sqrt{2.032(\kappa-1) \left(\frac{0.73 \operatorname{Tr}(G)}{t} + \log(K) + \log(\epsilon^{-1}) \right)} + \sqrt{\frac{98.5 \kappa \operatorname{Tr}(G)}{t}}, \quad t \in \mathbb{R}_+,$$

where $\operatorname{Tr}(G) = \mathbb{E}[\|X\|^2]$ denotes the trace of the Gram matrix, and

$$B_*(t) = \begin{cases} \frac{n^{-1/2} \zeta_*(\max\{t, \sigma\})}{1 - 4n^{-1/2} \zeta_*(\max\{t, \sigma\})} & [6 + (\kappa-1)^{-1}] \zeta_*(\max\{t, \sigma\}) \leq \sqrt{n} \\ +\infty & \text{otherwise.} \end{cases}$$

With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$,

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\hat{N}(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq B_* \left[\|\theta\|^{-2} N(\theta) \right].$$

For the proof we refer to section 5.2. Remark that equation (5.19) of the proof provides a bound for any choice of the parameter $a > 0$ and that we reported here only the numerical value of the bound when $a = 1/2$ for the sake of simplicity.

Assuming any reasonable bound on the sample size we can bound the logarithmic factor $\log \log(n)$ hidden in $\log(K)$ with a relatively small constant. In particular, if we choose $n \leq 10^{20}$, we get $\log(K) \leq 4.35$.

Observe that the bound B_* does not depend explicitly on the dimension d of the ambient space. More specifically, the dimension has been replaced by the entropy term

$$\mathbf{Tr}(G) / \max \{ \|\theta\|^{-2} N(\theta), \sigma \}.$$

Moreover, we do not need to know the exact values of κ and $\mathbf{Tr}(G)$ to compute the estimator and evaluate the bound, it is sufficient to know upper bounds instead. Indeed, if we use those upper bounds to define our estimator, the above result is still true with κ and $\mathbf{Tr}(G)$ replaced by their upper bounds.

We also observe that in order to have a meaningful (finite) bound we can choose the threshold σ such that

$$8\zeta_*(\sigma) \leq \sqrt{n} \quad (2.13)$$

so that $B_*(t) < +\infty$ for any $t \in \mathbb{R}_+$, assuming that $\kappa \geq 3/2$. More precisely, using the inequality $(\sqrt{a} + \sqrt{b})^2 \leq 2(a + b)$, we see that equation (2.13) holds when

$$\sigma = \frac{100 \kappa \mathbf{Tr}(G)}{n/128 - 4.35 - \log(\epsilon^{-1})}.$$

With this choice the threshold σ decays to zero at speed $1/n$ as the sample size grows to infinity.

Remark that the estimator \hat{N} is not necessarily a quadratic form. We conclude this section by introducing and studying a quadratic estimator of N .

We observe that Proposition 2.1 provides a confidence region for $N(\theta)$. Define

$$B_-(\theta) = \max_{(\lambda, \beta) \in \Lambda} \Phi_- (\tilde{N}_\lambda(\theta)) \quad \text{and} \quad B_+(\theta) = \min_{(\lambda, \beta) \in \Lambda} \Phi_+^{-1} (\tilde{N}_\lambda(\theta))$$

where we recall that $\tilde{N}_\lambda(\theta) = \frac{\lambda}{\hat{\alpha}(\theta)^2}$ and Λ is defined in equation (2.11). According to Proposition 2.1, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$,

$$B_-(\theta) \leq N(\theta) \leq B_+(\theta). \quad (2.14)$$

From a theoretical point of view we can consider as an estimator of N any quadratic form belonging to the confidence interval $[B_-(\theta), B_+(\theta)]$ for any θ . Such a quadratic form exists with probability at least $1 - 2\epsilon$ according to equation (2.14). However, from an algorithmic point of view, we would like to impose these constraints only for a finite number of directions θ . In particular, in the

following we are going to study the properties of a symmetric matrix Q that satisfies $\text{Tr}(Q^2) \leq \text{Tr}(G^2)$ and

$$B_-(\theta) \leq \theta^\top Q \theta \leq B_+(\theta), \quad \theta \in \Theta_\delta,$$

where Θ_δ is any finite δ -net of the unit sphere $\mathbb{S}_d = \{\theta \in \mathbb{R}^d, \|\theta\| = 1\}$, meaning that

$$\sup_{\theta \in \mathbb{S}_d} \min_{\xi \in \Theta_\delta} \|\theta - \xi\| \leq \delta.$$

The matrix Q can be computed using a convex optimization algorithm as described in [Catoni, O. \(2015\)](#) or [Giulini, I. \(2015\)](#).

From now on let $\sigma \in]0, s_4^2]$ be a threshold such that $8\zeta_*(\sigma) \leq \sqrt{n}$. Next proposition provides the analogous for the quadratic form $\theta^\top Q \theta$ of the dimension-free bound presented in Proposition [2.3](#) for $\hat{N}(\theta)$.

Proposition 2.4. *With the same notation as in Proposition [2.3](#), with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$,*

$$\begin{aligned} \left| \max\{\theta^\top Q \theta, \sigma\} - \max\{N(\theta), \sigma\} \right| &\leq 2 \max\{N(\theta), \sigma\} B_*(N(\theta)) + 5\delta \sqrt{\text{Tr}(G^2)}, \\ \left| \max\{\theta^\top Q \theta, \sigma\} - \max\{N(\theta), \sigma\} \right| &\leq 2 \max\{\theta^\top Q \theta, \sigma\} B_*(\min\{\theta^\top Q \theta, s_4^2\}) + 5\delta \sqrt{\text{Tr}(G^2)}. \end{aligned}$$

Proof. Since for any $\theta \in \mathbb{S}_d$ there is $\xi \in \Theta_\delta$ such that $\|\theta - \xi\| \leq \delta$, we have

$$\begin{aligned} |\theta^\top Q \theta - \xi^\top Q \xi| &= (\theta + \xi)^\top Q (\theta - \xi) \\ &\leq \|\theta + \xi\| \|Q\|_\infty \|\theta - \xi\| \leq 2\delta \sqrt{\text{Tr}(Q^2)} \leq 2\delta \sqrt{\text{Tr}(G^2)}. \end{aligned} \quad (2.15)$$

Let us put $\eta = 2\delta \sqrt{\text{Tr}(G^2)}$. We observe that, with probability at least $1 - 2\epsilon$,

$$\begin{aligned} \Phi_- \circ \Phi_+(\theta^\top Q \theta - \eta) &\leq N(\theta) + \eta, \\ \Phi_- \circ \Phi_+(N(\theta) - \eta) &\leq \theta^\top Q \theta + \eta, \end{aligned} \quad (2.16)$$

where Φ_+ and Φ_- are defined in Proposition [2.1](#) and depend on θ only through $\|\theta\|$. Indeed, in the event of probability at least $1 - 2\epsilon$ described in equation [\(2.14\)](#),

$$\theta^\top Q \theta \leq \Phi_+^{-1}(\tilde{N}_\lambda(\xi)) + \eta \leq \Phi_+^{-1} \circ \Phi_-^{-1}(N(\xi)) + \eta \leq \Phi_+^{-1} \circ \Phi_-^{-1}(N(\theta) + \eta) + \eta,$$

since equation [\(2.15\)](#) also holds for N , and in the same way we get

$$\theta^\top Q \theta \geq \Phi_-(\tilde{N}_\lambda(\xi)) - \eta \geq \Phi_- \circ \Phi_+(N(\xi)) - \eta \geq \Phi_- \circ \Phi_+(N(\theta) - \eta) - \eta$$

which proves equation [\(2.16\)](#). According to Corollary [5.1](#) in section [5.4](#) we conclude the proof. \square

According to equation (2.15), for any $\theta \in \mathbb{S}_d$

$$|\theta^\top Q \theta - \xi^\top Q \xi| \leq 2\delta \sqrt{\text{Tr}(G^2)}$$

where $\xi \in \Theta_\delta$ is such that $\|\theta - \xi\| \leq \delta$. There is still some improvement to bring, since at this stage we are not sure that Q is non-negative. Decomposing Q into its positive and negative parts and writing $Q = Q_+ - Q_-$, we can consider as an estimator of G the positive semi-definite symmetric matrix Q_+ as shown in the following proposition.

Proposition 2.5. *With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$,*

$$\begin{aligned} \left| \max\{\theta^\top Q_+ \theta, \sigma\} - \max\{N(\theta), \sigma\} \right| &\leq 2 \max\{N(\theta), \sigma\} B_*(N(\theta)) + 7\delta \sqrt{\text{Tr}(G^2)}, \\ \left| \max\{\theta^\top Q_+ \theta, \sigma\} - \max\{N(\theta), \sigma\} \right| &\leq 2 \max\{\theta^\top Q_+ \theta, \sigma\} B_*(\min\{\theta^\top Q_+ \theta, s_4^2\}) \\ &\quad + 7\delta \sqrt{\text{Tr}(G^2)}, \end{aligned}$$

where B_* is defined in Proposition 2.3.

Proof. Let us put as before $\eta = 2\delta \sqrt{\text{Tr}(G^2)}$. For any $\theta \in \mathbb{S}_d$, there is $\xi \in \Theta_\delta$ such that $\|\theta - \xi\| \leq \delta$, so that, according to equation (2.15),

$$\theta^\top Q \theta \geq \xi^\top Q \xi - \eta \geq -\eta.$$

Then we deduce that

$$\|Q_-\|_\infty = \sup_{\theta \in \mathbb{S}_d} \theta^\top Q_- \theta = - \inf_{\theta \in \mathbb{S}_d} \theta^\top Q \theta \leq \eta.$$

Therefore, for any $\theta \in \mathbb{S}_d$,

$$\left| \max\{\theta^\top Q \theta, \sigma\} - \max\{\theta^\top Q_+ \theta, \sigma\} \right| \leq \left| \theta^\top Q \theta - \theta^\top Q_+ \theta \right| = \theta^\top Q_- \theta \leq \eta.$$

Combining the above equation with Proposition 2.4 we conclude the proof. \square

3. The infinite-dimensional setting

In this section we extend the results obtained in the previous section to the infinite-dimensional setting.

Let \mathcal{H} be a separable Hilbert space and let $P \in \mathcal{M}_+^1(\mathcal{H})$ be an unknown probability distribution on \mathcal{H} . We consider the Gram operator $\mathcal{G} : \mathcal{H} \rightarrow \mathcal{H}$ defined by

$$\mathcal{G}\theta = \int \langle \theta, v \rangle_{\mathcal{H}} v \, dP(v)$$

and we assume $\text{Tr}(\mathcal{G}) = \mathbb{E}(\|X\|_{\mathcal{H}}^2) < +\infty$, where $X \in \mathcal{H}$ denotes a random vector of law P . In analogy to the previous section we denote by N the quadratic form associated with the Gram operator \mathcal{G} so that

$$N(\theta) = \langle \mathcal{G}\theta, \theta \rangle_{\mathcal{H}} = \int \langle \theta, v \rangle_{\mathcal{H}}^2 \, dP(v), \quad \theta \in \mathcal{H}.$$

We consider $(\mathcal{H}_k)_k$ an increasing sequence of subspaces of \mathcal{H} of finite dimension such that $\bigcup_k \mathcal{H}_k = \mathcal{H}$ and we endow each space \mathcal{H}_k with the probability P_k which arises from the disintegration of P , meaning that, if Π_k is the orthogonal projector on \mathcal{H}_k , $P_k = P \circ \Pi_k^{-1}$. We denote by N_k the quadratic form in \mathcal{H}_k associated with the probability distribution P_k and we observe that, for any $\theta \in \mathcal{H}$, we have

$$N_k(\Pi_k \theta) = N(\Pi_k \theta).$$

In the following we consider i.i.d. samples of size n in \mathcal{H} drawn according to P . According to Proposition 2.1, the event

$$\mathcal{A}_k = \left\{ \forall \theta \in \mathcal{H}_k, \forall (\lambda, \beta) \in \Lambda, \Phi_{\theta, -} \left(\frac{\lambda}{\widehat{\alpha}(\theta)^2} \right) \leq N(\theta) \leq \Phi_{\theta, +}^{-1} \left(\frac{\lambda}{\widehat{\alpha}(\theta)^2} \right) \right\}$$

is such that $P^{\otimes n}(\mathcal{A}_k) \geq 1 - 2\epsilon$. Since $\mathcal{A}_{k+1} \subset \mathcal{A}_k$, by the continuity of measure,

$$P^{\otimes n} \left(\bigcap_{k \in \mathbb{N}} \mathcal{A}_k \right) \geq 1 - 2\epsilon.$$

This means that with probability at least $1 - 2\epsilon$, for any $\theta \in \bigcup_k \mathcal{H}_k$ and any $(\lambda, \beta) \in \Lambda$,

$$\Phi_{\theta, -} \left(\frac{\lambda}{\widehat{\alpha}(\theta)^2} \right) \leq N(\theta) \leq \Phi_{\theta, +}^{-1} \left(\frac{\lambda}{\widehat{\alpha}(\theta)^2} \right).$$

Consequently, since $N(\theta) = \lim_{k \rightarrow +\infty} N(\Pi_k(\theta))$, for any $\theta \in \mathcal{H}$, the following result holds.

Proposition 3.1. *With probability at least $1 - 2\epsilon$, for any $\theta \in \mathcal{H}$,*

$$B_-(\theta) \leq N(\theta) \leq B_+(\theta)$$

where

$$\begin{aligned} B_-(\theta) &= \lim_{k \rightarrow +\infty} \sup_{(\lambda, \beta) \in \Lambda} \sup_{\Phi_{\Pi_k(\theta), -}} \left(\frac{\lambda}{\widehat{\alpha}(\Pi_k(\theta))^2} \right), \\ B_+(\theta) &= \lim_{k \rightarrow +\infty} \inf_{(\lambda, \beta) \in \Lambda} \inf_{\Phi_{\Pi_k(\theta), +}^{-1}} \left(\frac{\lambda}{\widehat{\alpha}(\Pi_k(\theta))^2} \right). \end{aligned}$$

If we do not want to go to the limit, we can use the explicit bound

$$\begin{aligned} |N(\theta) - N(\Pi_k(\theta))| &= |\langle \theta + \Pi_k(\theta), \mathcal{G}(\theta - \Pi_k(\theta)) \rangle_{\mathcal{H}}| \\ &\leq 2\|\theta\|_{\mathcal{H}} \|\mathcal{G}\|_{\infty} \|\theta - \Pi_k(\theta)\|_{\mathcal{H}} \leq 2\|\theta\|_{\mathcal{H}} \mathbf{Tr}(\mathcal{G}) \|\theta - \Pi_k(\theta)\|_{\mathcal{H}} \\ &= 2\|\theta\|_{\mathcal{H}} \mathbb{E}(\|X\|_{\mathcal{H}}^2) \|\theta - \Pi_k(\theta)\|_{\mathcal{H}}. \end{aligned}$$

This bound depends on $\|\theta - \Pi_k \theta\|_{\mathcal{H}}$. We will see in the following another bound that goes uniformly to zero for any $\theta \in \mathbb{S}_{\mathcal{H}}$ when k tends to infinity. In the same way, proceeding as already done in the previous section we state the analogous of Proposition 2.3.

Proposition 3.2. *Let*

$$\kappa \geq \sup_{\substack{\theta \in \mathcal{H} \\ \mathbb{E}(\langle \theta, X \rangle_{\mathcal{H}}^2) > 0}} \frac{\mathbb{E}(\langle \theta, X \rangle_{\mathcal{H}}^4)}{\mathbb{E}(\langle \theta, X \rangle_{\mathcal{H}}^2)^2} \quad \text{and} \quad s_4 \geq \mathbb{E}(\|X\|_{\mathcal{H}}^4)^{1/4}$$

be known constants and put

$$K = 1 + \left\lceil 2 \log \left(\frac{n}{72(2+c)\kappa^{1/2}} \right) \right\rceil$$

where $c = \frac{15}{8 \log(2)(\sqrt{2}-1)} \exp \left(\frac{1+2\sqrt{2}}{2} \right)$. *Define*

$$\zeta_*(t) = \sqrt{2.032(\kappa-1) \left(\frac{0.73 \text{Tr}(\mathcal{G})}{t} + \log(K) + \log(\epsilon^{-1}) \right)} + \sqrt{\frac{98.5\kappa \text{Tr}(\mathcal{G})}{t}}$$

and consider, according to equation (2.12), the estimator

$$\hat{N}(\theta) = \tilde{N}_{\hat{\lambda}}(\theta), \quad \theta \in \bigcup_k \mathcal{H}_k.$$

For any $\theta \in \mathcal{H}$, *define* $\hat{N}(\theta)$ *by choosing any accumulation point of the sequence* $\hat{N}(\Pi_k(\theta))$. *Define the bound*

$$B_*(t) = \frac{n^{-1/2} \zeta_*(\max\{t, \sigma\})}{1 - 4n^{-1/2} \zeta_*(\max\{t, \sigma\})},$$

where $\sigma \in]0, s_4^2]$ *is some energy level such that*

$$[6 + (\kappa - 1)^{-1}] \zeta_*(\sigma) \leq \sqrt{n}.$$

With probability at least $1 - 2\epsilon$, *for any* $\theta \in \mathcal{H}$,

$$\left| \frac{\max\{N(\theta), \sigma \|\theta\|_{\mathcal{H}}^2\}}{\max\{\hat{N}(\theta), \sigma \|\theta\|_{\mathcal{H}}^2\}} - 1 \right| \leq B_* \left[\|\theta\|_{\mathcal{H}}^{-2} N(\theta) \right].$$

Proof. This is a consequence of the fact that $\lim_{k \rightarrow +\infty} N(\Pi_k(\theta)) = N(\theta)$ and of the continuity of B_* . \square

As already discuss at the end of Proposition 2.3, any reasonable bound on the sample size n allows bounding the logarithmic factor $\log(K)$ by a relatively small constant. In particular, putting $n \leq 10^{20}$, we get $\log(K) \leq 4.35$.

In the following we construct an estimator of the Gram operator \mathcal{G} . Let $X_1, \dots, X_n \in \mathcal{H}$ be an i.i.d. sample drawn according to P . Define $V = \overline{\text{span}}\{X_1, \dots, X_n\}$ and

$$V_k = \overline{\text{span}}\{\Pi_k X_1, \dots, \Pi_k X_n\} = \Pi_k(V).$$

Let Θ_δ be a δ -net of $\mathbb{S}_{\mathcal{H}} \cap V_k$ (where $\mathbb{S}_{\mathcal{H}}$ denotes the unit sphere in \mathcal{H}) and remark that Θ_δ is finite because $\dim(V_k) \leq n < +\infty$. We compute a linear operator $\widehat{\mathcal{G}}_k : V_k \rightarrow V_k$ such that $\mathbf{Tr}(\widehat{\mathcal{G}}_k^2) \leq \mathbf{Tr}(\mathcal{G}^2)$ and

$$\Phi_-(\widetilde{N}_\lambda(\theta)) \leq \langle \widehat{\mathcal{G}}_k \theta, \theta \rangle_{\mathcal{H}} \leq \Phi_+^{-1}(\widetilde{N}_\lambda(\theta)), \quad \theta \in \Theta_\delta.$$

Observe that $\widehat{\mathcal{G}}_k$ plays the same role as the symmetric matrix \widehat{G} in the finite-dimensional setting. We consider as an estimator of \mathcal{G} the operator

$$\mathcal{Q} = \widehat{\mathcal{G}}_k \circ \Pi_{V_k}, \quad (3.1)$$

where Π_{V_k} is the orthogonal projector on V_k . Let us decompose \mathcal{Q} in its positive and negative parts and write $\mathcal{Q} = \mathcal{Q}_+ - \mathcal{Q}_-$.

Proposition 3.3. *For any threshold $\sigma \in \mathbb{R}_+$ such that $\sigma \leq s_4^2$ and $8\zeta_*(\sigma) \leq \sqrt{n}$, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_{\mathcal{H}}$ and for any k ,*

$$\begin{aligned} & \left| \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \Pi_k \theta, \mathcal{G} \Pi_k \theta \rangle_{\mathcal{H}}, \sigma\} \right| \\ & \leq 2 \max\{\langle \Pi_k \theta, \mathcal{G} \Pi_k \theta \rangle_{\mathcal{H}}, \sigma\} B_*(\langle \Pi_k \theta, \mathcal{G} \Pi_k \theta \rangle_{\mathcal{H}}) + 7\delta \sqrt{\mathbf{Tr}(\mathcal{G}^2)} \\ & \left| \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \Pi_k \theta, \mathcal{G} \Pi_k \theta \rangle_{\mathcal{H}}, \sigma\} \right| \\ & \leq 2 \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} B_*(\min\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, s_4^2\}) + 7\delta \sqrt{\mathbf{Tr}(\mathcal{G}^2)}. \end{aligned}$$

For the proof we refer to section 5.3.

Let us consider $\{p_i\}_{i=1}^{+\infty}$ an orthonormal basis of eigenvectors of \mathcal{G} such that the corresponding sequence of eigenvalues $\{\lambda_i, i = 1, \dots, +\infty\}$ is non-increasing.

Proposition 3.4. *Consider some threshold $\sigma \in \mathbb{R}_+$ such that $\sigma \leq s_4^2$ and $8\zeta_*(\sigma) \leq \sqrt{n}$. With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_{\mathcal{H}}$ and for any k ,*

$$\begin{aligned} & \left| \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \theta, \mathcal{G} \theta \rangle_{\mathcal{H}}, \sigma\} \right| \leq 2 \max\{\langle \theta, \mathcal{G} \theta \rangle_{\mathcal{H}}, \sigma\} B_*(\langle \theta, \mathcal{G} \theta \rangle_{\mathcal{H}}) \\ & \quad + 7\delta \sqrt{\mathbf{Tr}(\mathcal{G}^2)} + 3\nu_k \\ & \left| \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \theta, \mathcal{G} \theta \rangle_{\mathcal{H}}, \sigma\} \right| \leq 2 \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} B_*(\min\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, s_4^2\}) \\ & \quad + 7\delta \sqrt{\mathbf{Tr}(\mathcal{G}^2)} + 2\nu_k, \end{aligned}$$

where

$$\begin{aligned} \nu_k &= \inf_{m=1, \dots, +\infty} \left(\sum_{i=1}^{m-1} \lambda_i \|p_i - \Pi_k p_i\|_{\mathcal{H}} + \lambda_m/2 \right) \\ &\leq \inf_{m=1, \dots, +\infty} \left(\sum_{i=1}^{m-1} \lambda_i \|p_i - \Pi_k p_i\|_{\mathcal{H}} + \mathbf{Tr}(\mathcal{G})/(2m) \right) \xrightarrow{k \rightarrow +\infty} 0. \end{aligned}$$

Proof. It is enough to observe that

$$\begin{aligned} & \left| \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \theta, \mathcal{G} \theta \rangle_{\mathcal{H}}, \sigma\} \right| \\ & \leq \left| \max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \Pi_k \theta, \mathcal{G} \Pi_k \theta \rangle_{\mathcal{H}}, \sigma\} \right| + \left| \langle \theta, \mathcal{G} \theta \rangle_{\mathcal{H}} - \langle \Pi_k \theta, \mathcal{G} \Pi_k \theta \rangle_{\mathcal{H}} \right| \end{aligned}$$

and, for any $\theta \in \mathbb{S}_{\mathcal{H}}$, we have

$$\begin{aligned} |\langle \theta, \mathcal{G}\theta \rangle_{\mathcal{H}} - \langle \Pi_k \theta, \mathcal{G}\Pi_k \theta \rangle_{\mathcal{H}}| &= \left| \sum_{i=1}^{+\infty} (\langle \Pi_k \theta, p_i \rangle_{\mathcal{H}}^2 - \langle \theta, p_i \rangle_{\mathcal{H}}^2) \lambda_i \right| \\ &= \left| \sum_{i=1}^{+\infty} (\langle \theta, \Pi_k p_i \rangle_{\mathcal{H}}^2 - \langle \theta, p_i \rangle_{\mathcal{H}}^2) \lambda_i \right| = \left| \sum_{i=1}^{+\infty} \langle \theta, \Pi_k p_i + p_i \rangle_{\mathcal{H}} \langle \theta, p_i - \Pi_k p_i \rangle_{\mathcal{H}} \lambda_i \right| \\ &\leq \inf_{m=1, \dots, +\infty} \left(\sum_{i=1}^{m-1} 2\lambda_i \|p_i - \Pi_k p_i\|_{\mathcal{H}} + \lambda_m \right). \end{aligned}$$

Indeed, $\sum_{i=m}^{+\infty} \langle \Pi_k \theta, p_i \rangle_{\mathcal{H}}^2 \leq 1$, so that

$$\sum_{i=m}^{+\infty} \langle \Pi_k \theta, p_i \rangle_{\mathcal{H}}^2 \lambda_i \leq \sup_{i=m, \dots, +\infty} \lambda_i = \lambda_m,$$

and in the same way

$$\sum_{i=m}^{+\infty} \langle \theta, p_i \rangle_{\mathcal{H}}^2 \lambda_i \leq \lambda_m.$$

□

Remark that we can use this result to bound $|\langle \theta, (\mathcal{G} - \mathcal{Q}_+) \theta \rangle_{\mathcal{H}}|$, using the inequality

$$|\langle \theta, (\mathcal{G} - \mathcal{Q}_+) \theta \rangle_{\mathcal{H}}| \leq |\max\{\langle \theta, \mathcal{Q}_+ \theta \rangle_{\mathcal{H}}, \sigma\} - \max\{\langle \theta, \mathcal{G}\theta \rangle_{\mathcal{H}}, \sigma\}| + \sigma.$$

Let us mention to conclude this section another way to extend the results from finite dimension to separable Hilbert spaces. This second method consists in defining directly a Gaussian perturbation of the parameter in the Hilbert space. Indeed, taking a basis, we can identify any separable Hilbert space \mathcal{H} with the sequence space $\ell^2 \subset \mathbb{R}^{\mathbb{N}}$. We can take as our prior parameter distribution π_0 the law on $\mathbb{R}^{\mathbb{N}}$ of a sequence of independent one-dimensional Gaussian random variables with mean 0 and variance $1/\beta$. For any $\theta \in \ell^2$, we can then define the posterior π_{θ} as $\bigotimes_{i \in \mathbb{N}} \mathcal{N}(\theta_i, 1/\beta) \in \mathcal{M}_+^1(\mathbb{R}^{\mathbb{N}})$. One can prove that

$$\mathcal{K}(\pi_{\theta}, \pi_0) = \sum_{i=1}^{+\infty} \mathcal{K}\left(\mathcal{N}((\theta_i, \beta^{-1}), \mathcal{N}(0, \beta^{-1}))\right) = \sum_{i=1}^{+\infty} \frac{\beta}{2} \theta_i^2 = \frac{\beta \|\theta\|_{\mathcal{H}}^2}{2}.$$

Moreover, when $\theta' \sim \pi_{\theta}$,

$$W(x) = \lim_{n \rightarrow +\infty} \sum_{i=0}^n \theta'_i x_i, \quad x \in \ell^2,$$

exists π_θ -almost surely and is a Gaussian process indexed by $\ell^2 \simeq \mathcal{H}$, with mean

$$\mathbb{E}[W(x)] = \langle \theta, x \rangle_{\mathcal{H}}, \quad x \in \mathcal{H},$$

and covariance

$$\mathbb{E}[W(x)W(y)] - \mathbb{E}[W(x)]\mathbb{E}[W(y)] = \frac{1}{\beta} \langle x, y \rangle_{\mathcal{H}}, \quad x, y \in \mathcal{H}.$$

Using these properties, we can directly generalize to $\ell^2 \simeq \mathcal{H}$ the PAC-Bayesian bounds stated in \mathbb{R}^d in the previous section. Nevertheless, we thought it was interesting to study more explicitly how the infinite dimension case could be approximated by a finite dimension estimator, as done in this section.

4. Empirical results

We present some empirical results which show the performance of our robust estimator. We use here a simplified construction that does not lead exactly to the estimator Q , for which we have proved theoretical results in the previous section, but should nonetheless exhibit the same kind of behavior.

We use an iterative scheme based on the polarization formula to estimate the coefficients of the Gram matrix in an orthonormal basis of eigenvectors and then update this basis iteratively to a basis of eigenvectors of the current estimate.

Let $X_1, \dots, X_n \in \mathbb{R}^d$ be a sample drawn according to the probability distribution P and let $\lambda > 0$. Let $p \in \mathbb{R}^n$ and define $S(p, \lambda)$ as the solution of

$$\sum_{i=1}^n \psi \left[\lambda \left(S(p, \lambda)^{-1} p_i^2 - 1 \right) \right] = 0.$$

In practice we compute $S(p, \lambda)$ using the Newton algorithm. We observe that, when $p_i = \langle \theta, X_i \rangle^2$ and λ is suitably chosen, $S(p, \lambda)$ is an approximation of the estimator $\hat{N}(\theta)$ of the quadratic form $N(\theta)$.

Define $S(p)$ as the solution obtained when the parameter λ is set to

$$\lambda = m \sqrt{\frac{1}{v} \left[\frac{2}{n} \log(\epsilon^{-1}) \left(1 - \frac{2}{n} \log(\epsilon^{-1}) \right) \right]}$$

where $m = \frac{1}{n} \sum_{i=1}^n p_i^2$, $v = \frac{1}{n-1} \sum_{i=1}^n (p_i^2 - m)^2$ and $\epsilon = 0.1$.

According to [Catoni, O. \(2012\)](#), this value of the scale parameter λ should be close to optimal for the estimation of a single expectation from an empirical sample distribution.

Let $\bar{\lambda}_1 \geq \dots \geq \bar{\lambda}_d \geq 0$ be the eigenvalues of the empirical Gram matrix \bar{G} , that will be our starting point, and let u_1, \dots, u_d be a corresponding orthonormal basis of eigenvectors. We decompose the empirical Gram matrix as

$$\bar{G} = UDU^\top$$

where U is the orthogonal matrix whose columns are the eigenvectors of \bar{G} and D is the diagonal matrix $D = \text{diag}(\bar{\lambda}_1, \dots, \bar{\lambda}_d)$. We observe that, by the polarization formula,

$$u_i^\top G u_j = \frac{1}{4} [N(u_i + u_j) - N(u_i - u_j)], \quad i, j = 1, \dots, d,$$

where $N(u_i + \sigma u_j)$, with $\sigma \in \{+1, -1\}$, is approximated by

$$S(\langle u_i + \sigma u_j, X_\ell \rangle^2, 1 \leq \ell \leq n).$$

Taking notation, for any $n \times d$ matrix W , we define $C(W)$ as the $d \times d$ matrix of entries

$$C(W)_{i,j} = \frac{1}{4} \left[S\left((W_{\ell,i} + W_{\ell,j})^2 \mid 1 \leq \ell \leq n\right) - S\left((W_{\ell,i} - W_{\ell,j})^2 \mid 1 \leq \ell \leq n\right) \right].$$

Let Y be the matrix whose i -th row is the vector X_i , so that

$$(YU)_{\ell,k} = \langle u_k, X_\ell \rangle, \quad 1 \leq \ell \leq n, \quad 1 \leq k \leq d.$$

We update the Gram matrix estimate to

$$Q_0 = UC(YU)U^\top.$$

Then we iterate the update scheme, decomposing Q_0 as

$$Q_0 = O_0 D_0 O_0^\top,$$

where $O_0 O_0^\top = O_0^\top O_0 = \mathbf{I}$ and D_0 is a diagonal matrix and computing

$$Q_1 = O_0 C(Y O_0) O_0^\top.$$

The inductive update step is more generally the following. Assuming we have constructed Q_k , we decompose it as

$$Q_k = O_k D_k O_k^\top$$

where $O_k O_k^\top = O_k^\top O_k = \mathbf{I}$ and D_k is a diagonal matrix and we define the new updated estimator of G as

$$Q_{k+1} = O_k C(Y O_k) O_k^\top.$$

We stop this iterative estimation scheme when $\|Q_k - Q_{k-1}\|_F$ falls under a given threshold. In the following numerical experiment we more simply performed four updates. We take as our robust estimator of G the last update Q_k .

We now present an example of the performance of this estimator, for some i.i.d. sample of size $n = 100$ in \mathbb{R}^{10} drawn according to the Gaussian mixture distribution

$$P = (1 - \alpha) \mathcal{N}(0, M_1) + \alpha \mathcal{N}(0, 16 \mathbf{I}),$$

where $\alpha = 0.05$ and

$$M_1 = \begin{bmatrix} 2 & 1 & & & 0 \\ 1 & 1 & & & \\ \hline & & 0.01 & & \\ 0 & & & \ddots & 0 \\ & & & 0 & 0.01 \end{bmatrix}.$$

The Gram matrix of P is equal to

$$G = (1 - \alpha)M_1 + 16\alpha\mathbf{I} = \begin{bmatrix} 2,7 & 0,95 & & & 0 \\ 0,95 & 1,75 & & & \\ \hline & & 0,8095 & & \\ 0 & & & \ddots & 0 \\ & & & 0 & 0,8095 \end{bmatrix}.$$

This example illustrates a favorable situation where the performance of the robust estimator is particularly striking when compared to the empirical Gram matrix. As it can be seen on the expression of the sample distribution as well as on the configuration plots below, this is a situation of intermittent high variance : the sample is a mixture of a rare high variance signal and a frequent low variance more structured signal.

We tested the algorithm on 500 different samples drawn according to the Gaussian mixture distribution defined above. Random sample configurations are presented in figure 1.

Figure 2 shows that the robust estimator Q significantly improves the error in terms of square of the Frobenius norm when compared to the empirical estimator \bar{G} . The red solid line represents the empirical quantile function of the errors of the robust estimator, whereas the blue dotted line represents the quantiles of $\|\bar{G} - G\|_F^2$.

This quantile function is obtained by sorting the 500 empirical errors in increasing order.

The mean of the square distances $\|Q - G\|_F^2$ on 500 trials is 5.6 ± 0.4 , where the indicated mean estimator and confidence interval is the non-asymptotic confidence interval given by Proposition 2.4 of Catoni, O. (2012) at confidence level 0.99. In the case of the empirical estimator, the mean is 15.5 ± 2 . The empirical standard deviations are respectively 2 and 10. So we see that in this case the robust estimator reliably decreases the error by a factor larger than 2 and also produces errors with a much smaller standard deviation from sample to sample.

In Appendix A we show from a theoretical point of view that the two estimators Q and \bar{G} behave in a similar way in light tail situations.

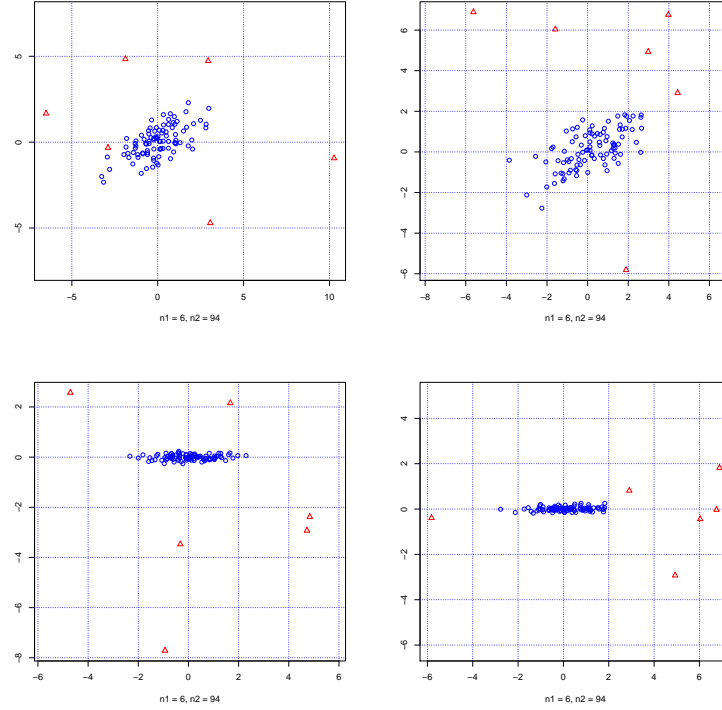


FIG 1. Two data samples projected onto the two first coordinates (above) and the second and third coordinates (below). Blue circles are drawn from the most frequent distribution and red triangles from the less frequent one.

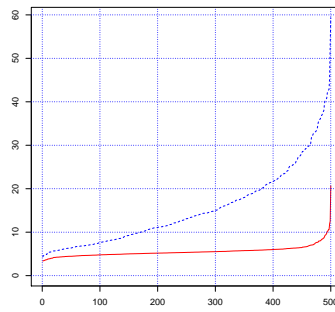


FIG 2. The red solid line represents the distances $\|Q - G\|_F^2$, the blue dotted line represents the distances $\|\bar{G} - G\|_F^2$.

5. Proofs

In this section we propose the proofs of the results presented in the previous sections. More precisely, section 5.1 refers to Proposition 2.1 (on page 6), section 5.2 refers to Proposition 2.3 (on page 7) and section 5.3 to Proposition 3.3 (on page 13). Finally section 5.4 is a (needed) technical section.

5.1. Proof of Proposition 2.1

The proof of Proposition 2.1 requires a sequence of preliminary results.

Our approach relies on perturbing the parameter θ with the Gaussian perturbation $\pi_\theta \sim \mathcal{N}(\theta, \beta^{-1}\mathbf{I})$, where $\beta > 0$ is a free parameter.

Lemma 5.1. *We have*

$$\int \langle \theta', x \rangle^2 d\pi_\theta(\theta') = \langle \theta, x \rangle^2 + \frac{\|x\|^2}{\beta}.$$

Proof. Let $W \in \mathbb{R}^d$ be a random variable drawn according to $\pi_\theta \sim \mathcal{N}(\theta, \beta^{-1}\mathbf{I})$. Therefore, $\langle W, x \rangle$ is one-dimensional Gaussian random variable with mean $\langle \theta, x \rangle$ and variance $x^\top (\beta^{-1}\mathbf{I})x = \frac{\|x\|^2}{\beta}$. Consequently

$$\int \langle \theta', x \rangle^2 d\pi_\theta(\theta') = \mathbb{E}[\langle W, x \rangle]^2 + \mathbf{Var}[\langle W, x \rangle] = \langle \theta, x \rangle^2 + \frac{\|x\|^2}{\beta}.$$

□

Accordingly we get

$$r_\lambda(\theta) = \frac{1}{n} \sum_{i=1}^n \psi \left[\int \left(\langle \theta', x \rangle^2 - \frac{\|x\|^2}{\beta} - \lambda \right) d\pi_\theta(\theta') \right].$$

In order to pull the expectation with respect to π_θ out of the influence function ψ , with a minimal loss of accuracy, we introduce the function

$$\chi(z) = \begin{cases} \psi(z) & z \leq z_1 \\ \psi(z_1) + p_1(z - z_1) - (z - z_1)^2/8 & z_1 \leq z \leq z_1 + 4p_1 \\ \psi(z_1) + 2p_1^2 & z \geq z_1 + 4p_1 \end{cases} \quad (5.1)$$

where $z_1 \in [0, 1]$ is such that $\psi''(z_1) = -1/4$ and p_1 is defined by the condition $p_1 = \psi'(z_1)$. Using the explicit expression of the first and second derivative of ψ , we get

$$z_1 = 1 - \sqrt{4\sqrt{2} - 5},$$

$$p_1 = \psi'(z_1) = \frac{\sqrt{4\sqrt{2} - 5}}{2(\sqrt{2} - 1)}$$

and $\sup \chi = \psi(z_1) + 2p_1^2 = -\log[2(\sqrt{2} - 1)] + \frac{1+2\sqrt{2}}{2}$.

Lemma 5.2. *For any $z \in \mathbb{R}$,*

$$\psi(z) \leq \chi(z) \leq \log(1 + z + z^2/2). \quad (5.2)$$

Proof. We first prove that $\psi(z) \leq \chi(z)$. The inequality is trivial for $z \leq z_1$, since $\chi(z) = \psi(z)$. For $z \in [z_1, z_1 + 4p_1]$, performing a Taylor expansion at z_1 , we obtain that

$$\begin{aligned} \psi(z) &= \psi(z_1) + p_1(z - z_1) - \frac{1}{8}(z - z_1)^2 + \int_{z_1}^z \frac{\psi'''(u)}{2}(z - u)^2 du \\ &\leq \psi(z_1) + p_1(z - z_1) - \frac{1}{8}(z - z_1)^2 = \chi(z), \end{aligned}$$

since $\psi'''(u) \leq 0$ for $u \in [0, 1]$. Finally we observe that, for any $z \geq z_1 + 4p_1$,

$$\chi(z) = \psi(z_1) + 2p_1^2 > \log(2) \geq \psi(z).$$

Let us now show that $\chi(z) \leq \log(1 + z + z^2/2)$. For $z \leq z_1$, we have already seen that the inequality is satisfied since $\chi(z) = \psi(z)$. Moreover we observe that the function

$$f(z) = \log(1 + z + z^2/2)$$

is such that $f(z_1) \geq \chi(z_1)$ and also $f'(z_1) \geq \chi'(z_1)$. Performing a Taylor expansion at z_1 , we get

$$\begin{aligned} f(z) &= f(z_1) + f'(z_1)(z - z_1) + \int_{z_1}^z f''(u)(z - u)^2 du \\ &\geq \chi(z_1) + \chi'(z_1)(z - z_1) + \inf f'' \frac{(z - z_1)^2}{2}. \end{aligned}$$

Since for any $t \in [z_1, z_1 + 4p_1]$,

$$\inf f'' = f''(\sqrt{3} - 1) = -1/4 = \chi''(t),$$

we deduce that

$$f(z) \geq \chi(z_1) + p_1(z - z_1) - \frac{1}{8}(z - z_1)^2 = \chi(z).$$

In particular, $f(z_1 + 4p_1) \geq \chi(z_1 + 4p_1)$. Recalling that f is an increasing function while χ is constant on the interval $[z_1 + 4p_1, +\infty[$, we conclude the proof. \square

Next lemma allows us to pull the expectation with respect to π_θ out of the function χ .

Lemma 5.3. *Let Θ be a measurable space. For any $\rho \in \mathcal{M}_+^1(\Theta)$ and any $h \in L_\rho^1(\Theta)$,*

$$\chi\left(\int h d\rho\right) \leq \int \chi(h) d\rho + \frac{1}{8}\mathbf{Var}(h d\rho), \quad (5.3)$$

where by definition

$$\mathbf{Var}(h \, d\rho) = \int \left(h(\theta) - \int h \, d\rho \right)^2 d\rho(\theta) \in \mathbb{R} \cup \{+\infty\}.$$

Moreover,

$$\psi\left(\int h \, d\rho\right) \leq \int \chi(h) \, d\rho + \min\left\{\log(4), \frac{1}{8}\mathbf{Var}(h \, d\rho)\right\}.$$

Proof. To prove equation (5.3) we observe that performing a Taylor expansion of the function χ at $z = \int h \, d\rho$

$$\chi[h(\theta)] \geq \chi(z) + (h(\theta) - z)\chi'(z) + \inf \chi'' \frac{(h(\theta) - z)^2}{2},$$

so that, recalling that $\inf \chi'' = -1/4$, we get

$$\begin{aligned} \int \chi[h(\theta)] \, d\rho(\theta) &\geq \chi\left(\int h \, d\rho\right) - \frac{1}{8} \int \left(h(\theta) - \int h \, d\rho\right)^2 d\rho(\theta) \\ &= \chi\left(\int h \, d\rho\right) - \frac{1}{8} \mathbf{Var}(h \, d\rho). \end{aligned}$$

Combining equation (5.3) with the fact that $\psi(z) \leq \chi(z)$, for any $z \in \mathbb{R}$, we obtain that

$$\psi\left(\int h \, d\rho\right) \leq \int \chi(h) \, d\rho + \frac{1}{8} \mathbf{Var}(h \, d\rho).$$

Moreover, since

$$\psi\left(\int h \, d\rho\right) - \int \chi(h) \, d\rho \leq \sup \psi - \inf \chi \leq \log(4),$$

we conclude the proof. \square

Applying this result to our problem we obtain

$$\begin{aligned} \psi(\langle \theta, x \rangle^2 - \lambda) &\leq \int \chi\left(\langle \theta', x \rangle^2 - \frac{\|x\|^2}{\beta} - \lambda\right) d\pi_\theta(\theta') \\ &\quad + \min\left\{\log(4), \frac{1}{8}\mathbf{Var}[\langle \theta', x \rangle^2 d\pi_\theta(\theta')]\right\}, \end{aligned}$$

where, putting $m = \langle \theta, x \rangle$, $\sigma = \frac{\|x\|}{\sqrt{\beta}}$ and denoting by $W \sim \mathcal{N}(0, \sigma^2)$ a centered Gaussian random variable,

$$\begin{aligned} \mathbf{Var}[\langle \theta', x \rangle^2 d\pi_\theta(\theta')] &= \mathbf{Var}[(m + W)^2] \\ &= 4m^2\sigma^2 + 2\sigma^4 = \frac{4\langle \theta, x \rangle^2 \|x\|^2}{\beta} + \frac{2\|x\|^4}{\beta^2}. \end{aligned}$$

Let us remark that, for any $a, b, c \in \mathbb{R}_+$ and $W \sim \mathcal{N}(0, \sigma^2)$,

$$\min\{a, bm^2 + c\} \leq \min\{a, b(m+W)^2 + c\} + \min\{a, b(m-W)^2 + c\}, \quad (5.4)$$

since $bm^2 + c \leq \max\{b(m+W)^2 + c, b(m-W)^2 + c\}$. Therefore, taking the expectation with respect to W of this inequality and remarking that W and $-W$ have the same probability distribution we get

$$\min\{a, bm^2 + c\} \leq 2\mathbb{E}\left[\min\{a, b(m+W)^2 + c\}\right].$$

Thus in our context we put $a = \log(4)$, $b = \|x\|^2/(2\beta)$ and $c = \|x\|^4/(4\beta^2)$ and we obtain

$$\begin{aligned} \psi(\langle \theta, x \rangle^2 - \lambda) &\leq \int \chi\left(\langle \theta', x \rangle^2 - \frac{\|x\|^2}{\beta} - \lambda\right) d\pi_\theta(\theta') \\ &\quad + \int \min\left\{4\log(2), \frac{\langle \theta', x \rangle^2 \|x\|^2}{\beta} + \frac{\|x\|^4}{2\beta^2}\right\} d\pi_\theta(\theta'). \end{aligned}$$

Lemma 5.4. *For any positive constants b, y and any $z \in \mathbb{R}$,*

$$\chi(z) + \min\{b, y\} \leq \log\left(1 + z + \frac{z^2}{2} + y \exp(\sup \chi) \frac{(\exp(b) - 1)}{b}\right).$$

Proof. For any positive real constants a, b, y ,

$$\begin{aligned} \log(a) + \min\{b, y\} &= \log(a \exp(\min\{b, y\})) \\ &\leq \log\left(a + a \min\{b, y\} \frac{(\exp(b) - 1)}{b}\right), \end{aligned}$$

since the function $x \mapsto \frac{e^x - 1}{x}$ is non-decreasing for $x \geq 0$. It follows that

$$\log(a) + \min\{b, y\} \leq \log[a + ya(\exp(b) - 1)/b].$$

Applying this inequality to $a = \exp[\chi(z)]$ and reminding that $\chi(z) \leq \log(1 + z + z^2/2)$, we conclude the proof. \square

As a consequence, choosing $b = 4\log(2)$, $z = \langle \theta', x \rangle^2 - \|x\|^2/\beta - \lambda$ and $y = \langle \theta', x \rangle^2 \|x\|^2/\beta + \|x\|^4/2\beta^2$, we get

$$\begin{aligned} \psi(\langle \theta, x \rangle^2 - \lambda) &\leq \int \log\left[1 + \langle \theta', x \rangle^2 - \frac{\|x\|^2}{\beta} - \lambda + \frac{1}{2}\left(\langle \theta', x \rangle^2 - \frac{\|x\|^2}{\beta} - \lambda\right)^2\right. \\ &\quad \left.+ \frac{c\|x\|^2}{\beta}\left(\langle \theta', x \rangle^2 + \frac{\|x\|^2}{2\beta}\right)\right] d\pi_\theta(\theta'), \end{aligned}$$

$$\text{where } c = \frac{15}{8\log(2)(\sqrt{2}-1)} \exp\left(\frac{1+2\sqrt{2}}{2}\right) \leq 44.3.$$

We observe that the above inequality allows to compare $\psi(\langle \theta, x \rangle^2 - \lambda)$ with the expectation with respect to the Gaussian perturbation π_θ . In terms of the empirical criterion r_λ we have proved that

$$r_\lambda(\theta) \leq \frac{1}{n} \sum_{i=1}^n \int \log \left[1 + \langle \theta', X_i \rangle^2 - \frac{\|X_i\|^2}{\beta} - \lambda + \frac{1}{2} \left(\langle \theta', X_i \rangle^2 - \frac{\|X_i\|^2}{\beta} - \lambda \right)^2 + \frac{c\|X_i\|^2}{\beta} \left(\langle \theta', X_i \rangle^2 + \frac{\|X_i\|^2}{2\beta} \right) \right] d\pi_\theta(\theta').$$

We are now ready to use the following general purpose PAC-Bayesian inequality.

Proposition 5.1. *Let $\nu \in \mathcal{M}_+^1(\mathbb{R}^d)$ be a prior probability distribution on \mathbb{R}^d and let $f : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [a, +\infty]$ be a measurable function with $a > -1$. With probability at least $1 - \epsilon$, for any posterior distribution $\rho \in \mathcal{M}_+^1(\mathbb{R}^d)$,*

$$\int \frac{1}{n} \sum_{i=1}^n f(X_i, \theta') d\rho(\theta') \leq \int \log \mathbb{E}[\exp(f(X, \theta'))] d\rho(\theta') + \frac{\mathcal{K}(\rho, \nu) + \log(\epsilon^{-1})}{n},$$

where

$$\mathcal{K}(\rho, \nu) = \begin{cases} \int \log \left(\frac{d\rho}{d\nu} \right) d\rho, & \text{if } \rho \ll \nu, \\ +\infty, & \text{otherwise,} \end{cases}$$

is the Kullback divergence of ρ with respect to ν . By convention, a non measurable event is said to happen with probability at least $1 - \epsilon$ when it includes a measurable event of probability non-smaller than $1 - \epsilon$.

For the proof we refer to (Catoni, O., 2012, page 1164) or Giulini, I. (2015).

In our context, we consider as prior distribution $\nu = \pi_0 = \mathcal{N}(0, \beta^{-1}\mathbf{I})$ and the family of posterior distributions consisting in the Gaussian perturbations

$$\{\pi_\theta \sim \mathcal{N}(\theta, \beta^{-1}\mathbf{I}) \mid \theta \in \mathbb{R}^d, \beta > 0\}$$

so that the Kullback divergence is given by

$$\mathcal{K}(\pi_\theta, \pi_0) = \frac{\beta\|\theta\|^2}{2}.$$

We observe that since the result holds for any choice of the posterior, it allows us to obtain uniform results in θ . More precisely, we apply the above PAC-Bayesian inequality to

$$f(X_i, \theta') = \log \left[1 + t(X_i, \theta') + \frac{1}{2}t(X_i, \theta')^2 + \frac{c\|X_i\|^2}{\beta} \left(\langle \theta', X_i \rangle + \frac{\|X_i\|^2}{2\beta} \right) \right],$$

where $t(x, \theta') = \langle \theta', x \rangle^2 - \frac{\|x\|^2}{\beta} - \lambda$. Using the fact that $\log(1+t) \leq t$, we get that, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{R}^d$,

$$\begin{aligned} r_\lambda(\theta) &\leq \int \mathbb{E} \left[t(X, \theta') + \frac{1}{2} t(X, \theta')^2 + \frac{c\|X\|^2}{\beta} \left(\langle \theta', X \rangle^2 + \frac{\|X\|^2}{2\beta} \right) \right] d\pi_\theta(\theta') \\ &\quad + \frac{\beta\|\theta\|^2}{2n} + \frac{\log(\epsilon^{-1})}{n} \\ &= \mathbb{E} \left[\langle \theta, X \rangle^2 - \lambda + \frac{1}{2} \left(\left(\langle \theta, X \rangle^2 - \lambda \right)^2 + \frac{4\langle \theta, X \rangle^2 \|X\|^2}{\beta} + \frac{2\|X\|^4}{\beta^2} \right) \right. \\ &\quad \left. + \frac{c\|X\|^2}{\beta} \left(\langle \theta, X \rangle^2 + \frac{3\|X\|^2}{2\beta} \right) \right] + \frac{\beta\|\theta\|^2}{2n} + \frac{\log(\epsilon^{-1})}{n}. \end{aligned}$$

To obtain the last line we have used the fact that

$$\begin{aligned} \int \langle \theta', X \rangle^2 d\pi_\theta(\theta') &= \langle \theta, X \rangle^2 + \frac{\|X\|^2}{\beta}, \\ \text{Var}[\langle \theta', X \rangle^2 d\pi_\theta(\theta')] &= \frac{4\langle \theta, X \rangle^2 \|X\|^2}{\beta} + \frac{2\|X\|^4}{\beta}. \end{aligned}$$

Let us recall the definition of s_4 and κ introduced in equation (2.5). We have defined

$$s_4 = \mathbb{E}[\|X\|^4]^{1/4} \quad \text{and} \quad \kappa = \sup_{\substack{\theta \in \mathbb{R}^d \\ \mathbb{E}[\langle \theta, X \rangle^2] > 0}} \frac{\mathbb{E}[\langle \theta, X \rangle^4]}{\mathbb{E}[\langle \theta, X \rangle^2]^2}.$$

Using the Cauchy-Schwarz inequality, since

$$\begin{aligned} \mathbb{E}[\langle \theta, X \rangle^4] &\leq \kappa N(\theta)^2 \\ \mathbb{E}[\langle \theta, X \rangle^2 \|X\|^2] &\leq \kappa^{1/2} s_4^2 N(\theta), \end{aligned}$$

we get that, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{R}^d$,

$$\begin{aligned} r_\lambda(\theta) &\leq \frac{\kappa}{2} [N(\theta) - \lambda]^2 + \left[1 + (\kappa - 1)\lambda + \frac{(2+c)\kappa^{1/2}s_4^2}{\beta} \right] [N(\theta) - \lambda] \\ &\quad + \frac{(\kappa - 1)\lambda^2}{2} + \frac{(2+c)\kappa^{1/2}s_4^2\lambda}{\beta} + \frac{(2+3c)s_4^4}{2\beta^2} + \frac{\beta\|\theta\|^2}{2n} + \frac{\log(\epsilon^{-1})}{n}. \end{aligned} \quad (5.5)$$

According to the (compact) notation introduced in equation (2.6), the above inequality rewrites as

$$\frac{r_\lambda(\theta)}{\lambda} \leq \xi \left(\frac{N(\theta)}{\lambda} - 1 \right)^2 + (1 + \mu) \left(\frac{N(\theta)}{\lambda} - 1 \right) + \gamma + \delta \|\theta\|^2. \quad (5.6)$$

Similarly, observing that

$$-r_\lambda(\theta) = \frac{1}{n} \sum_{i=1}^n \psi(\lambda - \langle \theta, X_i \rangle^2),$$

we obtain a lower bound for the empirical criterion r_λ . Namely, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{R}^d$, any $(\lambda, \beta) \in \Lambda$,

$$\frac{r_\lambda(\theta)}{\lambda} \geq -\xi \left(\frac{N(\theta)}{\lambda} - 1 \right)^2 + (1 - \mu) \left(\frac{N(\theta)}{\lambda} - 1 \right) - \gamma - \delta \|\theta\|^2. \quad (5.7)$$

We now combine the two bounds above to get the confidence region for $N(\theta)$ defined in Proposition 2.1. Assume that both equation (5.6) and equation (5.7) hold for any $\theta \in \mathbb{R}^d$, an event that happens with probability at least $1 - 2\epsilon$.

Let us introduce $\tau(\theta) = \frac{\lambda \delta \|\theta\|^2}{N(\theta)}$ and

$$p_\theta(z) = -\xi z^2 + [1 - \mu - \tau(\theta)] z - \gamma - \tau(\theta), \quad z \in \mathbb{R}.$$

We observe that $\tau(\alpha\theta) = \tau(\theta)$, and consequently $p_{\alpha\theta}(z) = p_\theta(z)$ for any $\alpha \in \mathbb{R}_+$. We consider the case when $p_\theta(1) > 0$, meaning that

$$\xi + \mu + \gamma + 2\tau(\theta) < 1. \quad (5.8)$$

In this case, the second degree polynomial p_θ has two distinct real roots, z_{-1} and z_{+1} , where

$$z_\sigma = \frac{1 - \mu - \tau(\theta) + \sigma \sqrt{[1 - \mu - \tau(\theta)]^2 - 4\xi[\gamma + \tau(\theta)]}}{2\xi}, \quad \sigma \in \{1, -1\}.$$

Since equation (5.8) can also be written as $-\xi > -[1 - \mu - \gamma - 2\tau(\theta)]$, we get

$$\begin{aligned} p_\theta \left(\frac{\gamma + \tau(\theta)}{1 - \mu - \gamma - 2\tau(\theta)} \right) \\ > \frac{-[\gamma + \tau(\theta)]^2}{1 - \mu - \gamma - 2\tau(\theta)} + [1 - \mu - \tau(\theta)] \frac{\gamma + \tau(\theta)}{1 - \mu - \gamma - 2\tau(\theta)} - \gamma - \tau(\theta) = 0, \end{aligned}$$

which implies

$$z_{-1} < \frac{\gamma + \tau(\theta)}{1 - \mu - \gamma - 2\tau(\theta)} < z_{+1}.$$

Therefore, since according to equation (5.7), for any $\alpha \in [0, \hat{\alpha}(\theta)]$,

$$p_\theta \left(\frac{\alpha^2 N(\theta)}{\lambda} - 1 \right) \leq \frac{r_\lambda(\alpha\theta)}{\lambda} \leq 0,$$

it holds that

$$\left[-1, \frac{\hat{\alpha}(\theta)^2 N(\theta)}{\lambda} - 1\right] \cap]z_{-1}, z_{+1}[= \emptyset.$$

Observing that $z_{-1} \geq 0 > -1$, it follows that $\hat{\alpha}(\theta)^2 N(\theta)/\lambda - 1 \leq z_{-1}$. This proves that, for any $\theta \in \mathbb{R}^d$ satisfying equation (5.8),

$$N(\theta) \leq \frac{\lambda}{\hat{\alpha}(\theta)^2} (1 + z_{-1}) \leq \frac{\lambda}{\hat{\alpha}(\theta)^2} \left(1 + \frac{\gamma + \tau(\theta)}{1 - \mu - \gamma - 2\tau(\theta)}\right),$$

which rewrites as

$$\Phi_{\theta,+}[N(\theta)] \leq \frac{\lambda}{\hat{\alpha}(\theta)^2}.$$

Moreover, this inequality is trivially true when condition (5.8) is not satisfied, because its left-hand side is equal to zero and its right-hand side is non-negative.

Proving the second part of the proposition requires a new argument and not a mere update of signs in the proof of the first part. Although it may seem at first sight that we are just aiming at a reverse inequality, the situation is more subtle than that.

Let us first remark that in the case when

$$\xi - \mu + \gamma + \delta \hat{\alpha}(\theta)^2 \|\theta\|^2 < 1, \quad (5.9)$$

is not satisfied, the bound

$$\Phi_{\theta,-}\left(\frac{\lambda}{\hat{\alpha}(\theta)^2}\right) \leq N(\theta) \quad (5.10)$$

is trivially satisfied because the left-hand side is equal to zero. In the case when equation (5.9) is true, it holds that $\hat{\alpha}(\theta) < +\infty$, so that $r_\lambda[\hat{\alpha}(\theta)\theta] = 0$, and therefore, according to equation (5.6),

$$0 \leq q_{\hat{\alpha}(\theta)\theta} \left(\frac{\hat{\alpha}(\theta)^2 N(\theta)}{\lambda} - 1 \right),$$

where $q_\theta(z) = \xi z^2 + (1 + \mu)z + \gamma + \delta \|\theta\|^2$.

Since condition (5.9) can also be written as $q_{\hat{\alpha}(\theta)\theta}(-1) < 0$, it implies that the second order polynomial $q_{\hat{\alpha}(\theta)\theta}$ has two roots and that $\frac{\hat{\alpha}(\theta)^2 N(\theta)}{\lambda} - 1$ is on the right of its largest root, which is larger than -1 . On the other hand, we observe that, under condition (5.9), putting $\hat{\tau}(\theta) = \delta \hat{\alpha}(\theta)^2 \|\theta\|^2$, we get

$$q_{\hat{\alpha}(\theta)\theta} \left(-\frac{\gamma + \hat{\tau}(\theta)}{1 + \mu - \gamma - \hat{\tau}(\theta)} \right) < \frac{(\gamma + \hat{\tau}(\theta))^2}{1 + \mu - \gamma - \hat{\tau}(\theta)} - \frac{(1 + \mu)[\gamma + \hat{\tau}(\theta)]}{1 + \mu - \gamma + \hat{\tau}(\theta)} + \gamma + \hat{\tau}(\theta) = 0.$$

Therefore, when condition (5.9) is satisfied,

$$\frac{\hat{\alpha}(\theta)^2 N(\theta)}{\lambda} - 1 \geq -\frac{\gamma + \hat{\tau}(\theta)}{1 + \mu - \gamma - \hat{\tau}(\theta)},$$

which rewrites as equation (5.10).

5.2. Proof of Proposition 2.3

We first observe that, according to Proposition 2.2, with probability at least $1 - 2\epsilon$,

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\widehat{N}(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq B_{\widehat{\lambda}, \widehat{\beta}} \left[\|\theta\|^{-2} \widehat{N}(\theta) \right] = \inf_{(\lambda, \beta) \in \Lambda} B_{\lambda, \beta} \left[\|\theta\|^{-2} \widetilde{N}_\lambda(\theta) \right]$$

since, by definition, $(\widehat{\lambda}, \widehat{\beta})$ are the values which minimize $B_{\lambda, \beta} \left[\|\theta\|^{-2} \widetilde{N}_\lambda(\theta) \right]$.

According to equation (2.9), since $\Phi_+(\|\theta\|^{-2} N(\theta)) \leq \|\theta\|^{-2} \widetilde{N}(\theta)$ and $B_{\lambda, \beta}$ is a decreasing function, we get

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\widehat{N}(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq \inf_{(\lambda, \beta) \in \Lambda} B_{\lambda, \beta} \left(\frac{\|\theta\|^{-2} N(\theta)}{1 + B_{\lambda, \beta} \left[\|\theta\|^{-2} N(\theta) \right]} \right).$$

With the same notation as in Proposition 2.2, we introduce the subset Γ' of Γ defined as

$$\Gamma' = \left\{ (\lambda, \beta, t) \in \Lambda \times \mathbb{R}_+ \mid \begin{aligned} &\xi + \mu + \gamma + 4\delta\lambda / \max\{t, \sigma\} < 1, \\ &\mu + \gamma + 2\delta\lambda / \max\{t, \sigma\} \leq 1/2, \\ &\text{and } 2\gamma + \delta\lambda / \max\{t, \sigma\} \leq 1/2 \end{aligned} \right\}$$

and the function

$$\widetilde{B}_{\lambda, \beta}(t) = \begin{cases} \frac{\gamma + \lambda\delta / \max\{t, \sigma\}}{1 - \mu - 2\gamma - 4\lambda\delta / \max\{t, \sigma\}}, & (\lambda, \beta, t) \in \Gamma', \\ +\infty, & \text{otherwise.} \end{cases} \quad (5.11)$$

Lemma 5.5. *For any $(\lambda, \beta) \in \Lambda$ and any $t \in \mathbb{R}_+$,*

$$\begin{aligned} B_{\lambda, \beta} \left(\frac{t}{1 + B_{\lambda, \beta}(t)} \right) &\leq \widetilde{B}_{\lambda, \beta}(t), \\ \frac{B_{\lambda, \beta}(t)}{1 - B_{\lambda, \beta}(t)} &\leq \widetilde{B}_{\lambda, \beta}(t). \end{aligned}$$

Proof. We first observe that when $(\lambda, \beta, t) \notin \Gamma'$ then $\widetilde{B}_{\lambda, \beta}(t) = +\infty$ and hence the two inequalities are trivial. We now assume $(\lambda, \beta, t) \in \Gamma'$ and we put $\tau = \lambda\delta / \max\{t, \sigma\}$. We prove the second inequality first. Since $\Gamma' \subset \Gamma$, we have

$$\frac{B_{\lambda, \beta}(t)}{1 - B_{\lambda, \beta}(t)} = \frac{\gamma + \tau}{1 - \mu - 2\gamma - 3\tau} \leq \widetilde{B}_{\lambda, \beta}(t).$$

In order to prove the first inequality, we first check that $(\lambda, \beta, \frac{t}{1 + B_{\lambda, \beta}(t)}) \in \Gamma$. We start observing that, since

$$\max\{t/[1 + B_{\lambda, \beta}(t)], \sigma\} \geq \max\{t, \sigma\}/[1 + B_{\lambda, \beta}(t)],$$

then

$$\begin{aligned}\xi + \mu + \gamma + 2\delta\lambda / \max\left\{\frac{t}{1+B_{\lambda,\beta}(t)}, \sigma\right\} &\leq \xi + \mu + \gamma + 2[1+B_{\lambda,\beta}(t)]\frac{\delta\lambda}{\max\{t, \sigma\}} \\ &= \xi + \mu + \gamma + 2\tau + 2\tau B_{\lambda,\beta}(t).\end{aligned}$$

Moreover, as $(\lambda, \beta, t) \in \Gamma'$, we get

$$B_{\lambda,\beta}(t) = \frac{\gamma + \tau}{1 - \mu - \gamma - 2\tau} \leq 1,$$

so that

$$\xi + \mu + \gamma + 2\delta\lambda / \max\{t/[1+B_{\lambda,\beta}(t)], \sigma\} \leq \xi + \mu + \gamma + 4\tau < 1,$$

which proves that, indeed, $(\lambda, \beta, \frac{t}{1+B_{\lambda,\beta}(t)}) \in \Gamma$. Therefore

$$\begin{aligned}B_{\lambda,\beta}\left(\frac{t}{1+B_{\lambda,\beta}(t)}\right) &\leq \frac{\gamma + \tau (1+B_{\lambda,\beta}(t))}{1 - \mu - \gamma - 2\tau[1 + \tau B_{\lambda,\beta}(t)]} \\ &= \frac{(\gamma + \tau)(1 + \tau/(1 - \mu - \gamma - 2\tau))}{1 - \mu - \gamma - 2\tau - 2\tau B_{\lambda,\beta}(t)},\end{aligned}$$

where in the last line we have used the definition of $B_{\lambda,\beta}$. Observing that

$$1 - \mu - \gamma - 2\tau - 2\tau B_{\lambda,\beta}(t) = \frac{(1 - \mu - \gamma - 2\tau)^2 - 2\tau(\gamma + \tau)}{1 - \mu - \gamma - 2\tau},$$

we obtain

$$\begin{aligned}B_{\lambda,\beta}\left(\frac{t}{1+B_{\lambda,\beta}(t)}\right) &\leq \frac{(\gamma + \tau)(1 - \mu - \gamma - \tau)}{(1 - \mu - \gamma - 2\tau)^2 - 2\tau(\gamma + \tau)} \\ &= \frac{(\gamma + \tau)(1 - \mu - \gamma - \tau)}{(1 - \mu - \gamma - \tau)^2 + \tau^2 - 2\tau(1 - \mu - \gamma - \tau) - 2\tau^2 - 2\gamma\tau} \\ &= \frac{\gamma + \tau}{1 - \mu - \gamma - \tau - 2\tau - (\tau^2 + 2\gamma\tau)/(1 - \mu - \gamma - \tau)}.\end{aligned}$$

Considering that

$$(\tau^2 + 2\gamma\tau) / (1 - \mu - \gamma - \tau) \leq \tau,$$

since when $(\lambda, \beta, t) \in \Gamma'$, it is true that $1 - \mu - \gamma - \tau \geq 1/2$ and $2\gamma + \tau \leq 1/2$, we conclude that

$$B_{\lambda,\beta}\left(\frac{t}{1+B_{\lambda,\beta}(t)}\right) \leq \frac{\gamma + \tau}{1 - \mu - \gamma - 4\tau} = \tilde{B}_{\lambda,\beta}(t).$$

□

Applying the above lemma to our problem we get that, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$,

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\widehat{N}(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq \inf_{(\lambda, \beta) \in \Lambda} \widetilde{B}_{\lambda, \beta}[\|\theta\|^{-2} N(\theta)]. \quad (5.12)$$

Let us recall the definition of the finite set Λ given in (2.11). Let $a > 0$ and

$$K = 1 + \left\lceil a^{-1} \log \left(\frac{n}{72(2+c)\kappa^{1/2}} \right) \right\rceil.$$

We define

$$\Lambda = \{(\lambda_j, \beta_j) \mid 0 \leq j < K\},$$

where

$$\begin{aligned} \lambda_j &= \sqrt{\frac{2}{n(\kappa-1)} \left(\frac{(2+3c)}{4(2+c)\kappa^{1/2} \exp(-ja)} + \log(K/\epsilon) \right)} \\ \beta_j &= \sqrt{2(2+c)\kappa^{1/2} s_4^4 n \exp[-(j-1/2)a]}. \end{aligned}$$

We introduce the explicit bound

$$\zeta(t) = \sqrt{2(\kappa-1) \left(\frac{(2+3c)s_4^2}{4(2+c)\kappa^{1/2}t} + \log(K/\epsilon) \right) \cosh(a/4) + \sqrt{\frac{2(2+c)\kappa^{1/2}s_4^2}{t}} \cosh(a/2)}$$

and

$$B_*(t) = \begin{cases} \frac{n^{-1/2}\zeta(\max\{t, \sigma\})}{1 - 4n^{-1/2}\zeta(\max\{t, \sigma\})} & [6 + (\kappa-1)^{-1}]\zeta(\max\{t, \sigma\}) \leq \sqrt{n} \\ +\infty & \text{otherwise.} \end{cases}$$

Lemma 5.6. *For any $t \in \mathbb{R}_+$, we have*

$$\inf_{(\lambda, \beta) \in \Lambda} \widetilde{B}_{\lambda, \beta}(t) \leq B_*(\min\{t, s_4^2\}). \quad (5.13)$$

Proof. We recall that the function $\widetilde{B}_{\lambda, \beta}$ is non-increasing so that $\widetilde{B}_{\lambda, \beta}(t) \leq \widetilde{B}_{\lambda, \beta}(\min\{t, s_4^2\})$. Moreover, since

$$\max\{\min\{t, s_4^2\}, \sigma\} = \min\{\max\{t, \sigma\}, s_4^2\},$$

it is sufficient to prove the result for $\max\{t, \sigma\} \in [0, s_4^2]$.

As equation (5.13) is trivial when $B_*(t) = +\infty$, we may assume that $B_*(t) < +\infty$, so that $6\zeta(\max\{t, \sigma\}) \leq \sqrt{n}$. In particular, by considering only the second term in the definition of ζ , we obtain that

$$\sqrt{\frac{2(2+c)\kappa^{1/2}s_4^2}{\max\{t, \sigma\}}} \leq \sqrt{\frac{2(2+c)\kappa^{1/2}s_4^2}{\max\{t, \sigma\}}} \cosh(a/2) \leq \frac{\sqrt{n}}{6},$$

which implies

$$\frac{\max\{t, \sigma\}}{s_4^2} \geq \frac{72(2+c)\kappa^{1/2}}{n} \geq \exp(-a(K-1)).$$

Therefore, since

$$\log\left(\frac{\max\{t, \sigma\}}{s_4^2}\right) \in [-a(K-1), 0],$$

there exists $\hat{j} \in \{0, \dots, K-1\}$ for which

$$\left| \log\left(\frac{\max\{t, \sigma\}}{s_4^2}\right) + \hat{j}a \right| \leq a/2. \quad (5.14)$$

We recall that by equation (2.6)

$$\gamma + \delta\lambda / \max\{t, \sigma\} = \frac{\lambda}{2}(\kappa-1) + \frac{(2+c)\kappa^{1/2}s_4^2}{\beta} + \frac{(2+3c)s_4^4}{2\beta^2\lambda} + \frac{\log(K/\epsilon)}{n\lambda} + \frac{\beta}{2n\max\{t, \sigma\}}$$

and we observe that (λ_*, β_*) defined as

$$\lambda_* = \sqrt{\frac{2}{n(\kappa-1)} \left(\frac{(2+3c)s_4^2}{4(2+c)k^{1/2}\max\{t, \sigma\}} + \log(K/\epsilon) \right)} \quad (5.15)$$

$$\beta_* = \sqrt{2(2+c)k^{1/2}s_4^2\max\{t, \sigma\}n} \quad (5.16)$$

are the desired values which optimize $\gamma + \delta\lambda / \max\{t, \sigma\}$. We also remark that, by equation (5.14),

$$\beta_{\hat{j}} \exp(-a/2) \leq \beta_* \leq \beta_{\hat{j}} \quad (5.17)$$

$$\lambda_{\hat{j}} \exp(-a/4) \leq \lambda_* \leq \lambda_{\hat{j}} \exp(a/4). \quad (5.18)$$

Thus, evaluating $\gamma + \delta\lambda / \max\{t, \sigma\}$ in $(\lambda_{\hat{j}}, \beta_{\hat{j}}) \in \Lambda$, we obtain that

$$\begin{aligned} & \gamma_{\hat{j}} + \delta_{\hat{j}}\lambda_{\hat{j}} / \max\{t, \sigma\} \\ &= \frac{\lambda_*(\kappa-1)}{2} \frac{\lambda_{\hat{j}}}{\lambda_*} + \frac{(2+c)\kappa^{1/2}s_4^2}{\beta_*} \frac{\beta_*}{\beta_{\hat{j}}} + \frac{(2+3c)s_4^4}{2\beta_{\hat{j}}^2\lambda_*} \frac{\lambda_*}{\lambda_{\hat{j}}} + \frac{\log(K/\epsilon)}{n\lambda_*} \frac{\lambda_*}{\lambda_{\hat{j}}} + \frac{\beta_*}{2n\max\{t, \sigma\}} \frac{\beta_{\hat{j}}}{\beta_*} \\ &\leq \frac{\lambda_*(\kappa-1)}{2} \frac{\lambda_{\hat{j}}}{\lambda_*} + \frac{1}{n\lambda_*} \left[\frac{(2+3c)s_4^2}{4(2+c)k^{1/2}\max\{t, \sigma\}} + \log(K/\epsilon) \right] \frac{\lambda_*}{\lambda_{\hat{j}}} \\ &\quad + \sqrt{\frac{(2+c)\kappa^{1/2}s_4^2}{2n\max\{t, \sigma\}}} \left(\frac{\beta_*}{\beta_{\hat{j}}} + \frac{\beta_{\hat{j}}}{\beta_*} \right) \\ &\leq \sqrt{\frac{2(\kappa-1)}{n} \left[\frac{(2+3c)s_4^2}{4(2+c)k^{1/2}\max\{t, \sigma\}} + \log(K/\epsilon) \right]} \cosh \left[\log \left(\frac{\lambda_{\hat{j}}}{\lambda_*} \right) \right] \\ &\quad + \sqrt{\frac{2(2+c)\kappa^{1/2}s_4^2}{n\max\{t, \sigma\}}} \cosh \left[\log \left(\frac{\beta_{\hat{j}}}{\beta_*} \right) \right]. \end{aligned}$$

By equation (5.17) we get

$$\begin{aligned} & \gamma_{\hat{\mathcal{J}}} + \delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\} \\ & \leq \sqrt{\frac{2(\kappa - 1)}{n} \left[\frac{(2 + 3c)s_4^2}{4(2 + c)k^{1/2} \max\{t, \sigma\}} + \log(K/\epsilon) \right] \cosh\left(\frac{a}{4}\right)} \\ & \quad + \sqrt{\frac{2(2 + c)\kappa^{1/2}s_4^2}{n \max\{t, \sigma\}} \cosh\left(\frac{a}{2}\right)}. \end{aligned}$$

We also observe that

$$\mu_{\hat{\mathcal{J}}} + \gamma_{\hat{\mathcal{J}}} + 4\delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\} \leq 4[\gamma_{\hat{\mathcal{J}}} + \delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\}] \leq 4n^{-1/2}\zeta(t),$$

since by definition $\mu_{\hat{\mathcal{J}}} \leq 2\gamma_{\hat{\mathcal{J}}}$. In the same way, observing that

$$\xi_{\hat{\mathcal{J}}} = \frac{\kappa \lambda_{\hat{\mathcal{J}}}}{2} \leq \gamma_{\hat{\mathcal{J}}} \left(1 + \frac{1}{\kappa - 1}\right)$$

we obtain

$$\begin{aligned} \xi_{\hat{\mathcal{J}}} + \mu_{\hat{\mathcal{J}}} + \gamma_{\hat{\mathcal{J}}} + 4\delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\} & < [4 + (\kappa - 1)^{-1}] \gamma_{\hat{\mathcal{J}}} + 4\delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\} \\ & \leq [6 + (\kappa - 1)^{-1}] n^{-1/2} \zeta(\max\{t, \sigma\}) \end{aligned}$$

and similarly,

$$\begin{aligned} 2[\mu_{\hat{\mathcal{J}}} + \gamma_{\hat{\mathcal{J}}} + 2\delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\}] & \leq 6n^{-1/2} \zeta(\max\{t, \sigma\}), \\ 2[2\gamma_{\hat{\mathcal{J}}} + \delta_{\hat{\mathcal{J}}} \lambda_{\hat{\mathcal{J}}} / \max\{t, \sigma\}] & \leq 4n^{-1/2} \zeta(\max\{t, \sigma\}). \end{aligned}$$

This implies that, whenever $B_*(t) < +\infty$, then $(\lambda_{\hat{\mathcal{J}}}, \beta_{\hat{\mathcal{J}}}, t) \in \Gamma'$. We have then proved that

$$\inf_{(\lambda, \beta) \in \Lambda} \tilde{B}_{\lambda, \beta}(t) \leq \tilde{B}_{\lambda_{\hat{\mathcal{J}}}, \beta_{\hat{\mathcal{J}}}}(t) \leq \frac{n^{-1/2} \zeta(\max\{t, \sigma\})}{1 - 4n^{-1/2} \zeta(\max\{t, \sigma\})} = B_*(t).$$

□

Applying the above lemma to equation (5.12) and observing that, for any $\theta \in \mathbb{R}^d$,

$$\|\theta\|^{-2} N(\theta) \leq \mathbb{E}[\|X\|^2] \leq s_4^2,$$

we obtain that, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$,

$$\left| \frac{\max\{N(\theta), \sigma \|\theta\|^2\}}{\max\{\hat{N}(\theta), \sigma \|\theta\|^2\}} - 1 \right| \leq B_*[\|\theta\|^{-2} N(\theta)].$$

Since by the Cauchy-Schwarz inequality

$$s_4^2 \leq \sqrt{\kappa} \mathbf{Tr}(G)$$

we get

$$\begin{aligned} \zeta(t) \leq & \sqrt{2(\kappa - 1) \left(\frac{(2 + 3c) \mathbf{Tr}(G)}{4(2 + c)t} + \log(K/\epsilon) \right) \cosh(a/4)} \\ & + \sqrt{\frac{2(2 + c)\kappa \mathbf{Tr}(G)}{t} \cosh(a/2)}. \end{aligned} \quad (5.19)$$

Choosing $a = 1/2$ and computing explicitly the constants we conclude the proof.

5.3. Proof of Proposition 3.3

We observe that it is sufficient to prove that with probability at least $1 - 2\epsilon$

$$\begin{aligned} \Phi_- \circ \Phi_+ \left(\langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}} - \eta \right) &\leq N(\Pi_k \theta) + \eta \\ \Phi_- \circ \Phi_+ \left(N(\Pi_k \theta) - \eta \right) &\leq \langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}} + \eta, \end{aligned} \quad (5.20)$$

where $\eta = 2\delta\sqrt{\mathbf{Tr}(\mathcal{G}^2)}$ and $N(\Pi_k \theta) = \langle \Pi_k \theta, \mathcal{G}\Pi_k \theta \rangle_{\mathcal{H}}$. Indeed, if equation (5.20) holds true, according to Corollary 5.1,

$$\begin{aligned} |\max\{\langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}}, \sigma\} - \max\{N(\Pi_k \theta), \sigma\}| &\leq 2 \max\{N(\Pi_k \theta), \sigma\} B_*(N(\Pi_k \theta)) + 5\eta/2 \\ |\max\{\langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}}, \sigma\} - \max\{N(\Pi_k \theta), \sigma\}| &\leq 2 \max\{\langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}}, \sigma\} B_*(\min\{\langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}}, s_4^2\}) \\ &\quad + 5\eta/2, \end{aligned}$$

which is the analogous, in the infinite-dimensional setting, of Proposition 2.4. Thus, following the proof of Proposition 2.5 we obtain the desired bounds.

Let us now prove equation (5.20). Observe that, for any $\theta \in \mathbb{S}_{\mathcal{H}}$,

$$\langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}} = \langle \Pi_{V_k} \theta, \mathcal{Q}\Pi_{V_k} \theta \rangle_{\mathcal{H}} \leq \|\Pi_{V_k} \theta\|_{\mathcal{H}}^2 (\langle \xi, \mathcal{Q}\xi \rangle_{\mathcal{H}} + \eta),$$

where $\xi \in \Theta_{\delta}$ is the closest point in Θ_{δ} to $\|\Pi_{V_k} \theta\|_{\mathcal{H}}^{-1} \Pi_{V_k} \theta$. Since $\xi \in \mathcal{H}_k$, with probability at least $1 - \epsilon$, for any $(\lambda, \beta) \in \Lambda$,

$$\langle \xi, \mathcal{Q}\xi \rangle_{\mathcal{H}} \leq \Phi_+^{-1}(\tilde{N}_{\lambda}(\xi)) = \Phi_+^{-1} \left[\tilde{N}_{\lambda} \left(\xi + \|\Pi_{V_k} \theta\|_{\mathcal{H}}^{-1} (\Pi_k - \Pi_{V_k}) \theta \right) \right].$$

Let us now remark that for any $a \in [0, 1]$, we have $\Phi_+(at) \leq a\Phi_+(t)$, so that $a\Phi_+^{-1}(t) \leq \Phi_+^{-1}(at)$. Therefore

$$\begin{aligned} \langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}} &\leq \|\Pi_{V_k} \theta\|_{\mathcal{H}}^2 \Phi_+^{-1} \left\{ \tilde{N}_{\lambda} \left[\|\Pi_{V_k} \theta\|_{\mathcal{H}}^{-1} \left(\|\Pi_{V_k} \theta\|_{\mathcal{H}} \xi + (\Pi_k - \Pi_{V_k}) \theta \right) \right] \right\} + \eta \\ &\leq \|\Pi_{V_k} \theta\|_{\mathcal{H}}^2 \Phi_+^{-1} \circ \Phi_-^{-1} \left\{ N \left[\|\Pi_{V_k} \theta\|_{\mathcal{H}}^{-1} \left(\|\Pi_{V_k} \theta\|_{\mathcal{H}} \xi + (\Pi_k - \Pi_{V_k}) \theta \right) \right] \right\} + \eta \\ &\leq \Phi_+^{-1} \circ \Phi_-^{-1} \left\{ N \left[\|\Pi_{V_k} \theta\|_{\mathcal{H}} \xi + (\Pi_k - \Pi_{V_k}) \theta \right] \right\} + \eta \\ &\leq \Phi_+^{-1} \circ \Phi_-^{-1} \left(N(\Pi_k \theta) + \eta \right) + \eta. \end{aligned}$$

Indeed,

$$\left\| \left(\|\Pi_{V_k}\theta\|_{\mathcal{H}}\xi + (\Pi_k - \Pi_{V_k})\theta \right) - \Pi_k\theta \right\| \leq \delta,$$

and this is a difference of two vectors belonging to the unit ball. In the same way

$$\begin{aligned} \langle \theta, \mathcal{Q}\theta \rangle_{\mathcal{H}} &\geq \|\Pi_{V_k}\theta\|_{\mathcal{H}}^2 (\langle \xi, \mathcal{Q}\xi \rangle_{\mathcal{H}} - \eta) \\ &\geq \|\Pi_{V_k}\theta\|_{\mathcal{H}}^2 \Phi_- \left\{ \tilde{N}_\lambda \left[\|\Pi_{V_k}\theta\|_{\mathcal{H}}^{-1} \left(\|\Pi_{V_k}\theta\|_{\mathcal{H}}\xi + (\Pi_k - \Pi_{V_k})\theta \right) \right] \right\} - \eta \\ &\geq \|\Pi_{V_k}\theta\|_{\mathcal{H}}^2 \Phi_- \circ \Phi_+ \left\{ N \left[\|\Pi_k\theta\|_{\mathcal{H}}^{-1} \left(\|\Pi_{V_k}\theta\|_{\mathcal{H}}\xi + (\Pi_k - \Pi_{V_k})\theta \right) \right] \right\} - \eta \\ &\geq \Phi_- \circ \Phi_+ \left(N(\Pi_k\theta) - \eta \right) - \eta \end{aligned}$$

which proves equation (5.20).

5.4. A technical result

In all this section we use the same notation as in section 2. Let $\sigma \in]0, s_4^2]$ be such that $8\zeta_*(\sigma) \leq \sqrt{n}$ where ζ_* is defined in Proposition 2.3.

Lemma 5.7. *The function*

$$t \mapsto F(t) = \max\{t, \sigma\} B_*(\min\{t, s_4^2\}),$$

where B_* is defined in Proposition 2.3, is non-decreasing for any $t \in \mathbb{R}_+$.

Proof. If $\sigma \geq s_4^2$, then $B_*(\min\{t, s_4^2\}) = B_*(\sigma)$, so that $F(t) = \max\{t, \sigma\} B_*(\sigma)$ is obviously non-decreasing. Otherwise, $\sigma \leq s_4^2$, so that

$$\zeta(\max\{\min\{t, s_4^2\}, \sigma\}) = \zeta(\min\{\max\{t, \sigma\}, s_4^2\}).$$

Therefore the function F is of the form

$$F(t) = c \frac{ug(u)}{(1 - g(u))},$$

where $u = \max\{t, \sigma\}$,

$$g(u) = \sqrt{a_1/u + a_2} + \sqrt{a_3/u},$$

$g(\sigma) \leq 1/2$, and the constants c, a_1, a_2 , and a_3 are positive. Let $h(u) = \sqrt{a_1/u} + \sqrt{a_3/u}$ and observe that

$$g'(u) = -\frac{1}{2u} \left(\frac{a_1/u}{(a_1/u + a_2)^{1/2}} + \sqrt{a_3/u} \right) \geq -\frac{1}{2u} \left(\sqrt{a_1/u} + \sqrt{a_3/u} \right) = h'(u)$$

and that $g(u) \geq h(u)$. Therefore $h(u) \leq g(u) \leq 1/2$, for any $u \geq \sigma$, and

$$\frac{\partial}{\partial u} \log \left(\frac{ug(u)}{1 - g(u)} \right) = \frac{1}{u} + \frac{g'(u)}{g(u)(1 - g(u))} \geq \frac{1}{u} + \frac{h'(u)}{h(u)(1 - h(u))} = \frac{1}{u} - \frac{1}{2u(1 - h(u))} \geq 0,$$

showing that F is non-decreasing. \square

Lemma 5.8. For any $(a, b) \in \mathbb{R}^2$ such that, for any $(\lambda, \beta) \in \Lambda$,

$$\Phi_- \circ \Phi_+(a - \eta) \leq b + \eta, \quad \text{and} \quad \Phi_- \circ \Phi_+(b - \eta) \leq a + \eta,$$

and any threshold $\sigma \in \mathbb{R}_+$ such that $8\zeta(\sigma) \leq \sqrt{n}$ and $\sigma \leq s_4^2$, we have

$$|\max\{a, \sigma\} - \max\{b, \sigma\}| \leq 2 \max\{a + \eta, \sigma\} B_*(\min\{a + \eta, s_4^2\}) + 2\eta \quad (5.21)$$

$$|\max\{a, \sigma\} - \max\{b, \sigma\}| \leq 2 \max\{b + \eta, \sigma\} B_*(\min\{b + \eta, s_4^2\}) + 2\eta. \quad (5.22)$$

Proof. By symmetry of a and b , equation (5.22) is a consequence of equation (5.21).

Step 1. We will prove that

$$\max\{b - \eta, \sigma\} \leq \max\{a + \eta, \sigma\} \left(1 + 2\tilde{B}_{\lambda, \beta}(a + \eta)\right), \quad (5.23)$$

where $\tilde{B}_{\lambda, \beta}$ is defined in equation (5.11).

Case 1. Assume that

$$\max\{\Phi_+(b - \eta), \sigma\} \leq \max\{a + \eta, \sigma\},$$

and remark that, since Φ_+ is non-decreasing and $\Phi_+(\sigma) \leq \sigma$,

$$\begin{aligned} \max\{\Phi_+(b - \eta), \sigma\} &\geq \max\{\Phi_+(b - \eta), \Phi_+(\sigma)\} \\ &= \Phi_+(\max\{(b - \eta), \sigma\}) = \frac{\max\{b - \eta, \sigma\}}{1 + B_{\lambda, \beta}(b - \eta)}, \end{aligned}$$

according to equation (2.9), where $B_{\lambda, \beta}$ is defined in equation (2.8). Therefore in this case,

$$\max\{b - \eta, \sigma\} \leq \max\{a + \eta, \sigma\} \left(1 + B_{\lambda, \beta}(b - \eta)\right), \quad (5.24)$$

but when $\max\{b - \eta, \sigma\} > \max\{a + \eta, \sigma\}$,

$$B_{\lambda, \beta}(b - \eta) \leq B_{\lambda, \beta}(a + \eta)$$

because $B_{\lambda, \beta}(t)$ is a non-increasing function of $\max\{t, \sigma\}$, thus equation (5.24) implies that

$$\max\{b - \eta, \sigma\} \leq \max\{a + \eta, \sigma\} \left(1 + B_{\lambda, \beta}(a + \eta)\right).$$

Since $B_{\lambda, \beta} \leq \tilde{B}_{\lambda, \beta}$, equation (5.23) holds true.

Case 2. Assume now that we are not in **Case 1**, implying that

$$\max\{b - \eta, \sigma\} \geq \max\{\Phi_+(b - \eta), \sigma\} > \max\{a + \eta, \sigma\}.$$

In this case

$$\begin{aligned} \max\{a + \eta, \sigma\} &\geq \max\{\Phi_- \circ \Phi_+(b - \eta), \sigma\} \geq \max\{\Phi_- \circ \Phi_+(b - \eta), \Phi_-(\sigma)\} \\ &\geq \Phi_-(\max\{\Phi_+(b - \eta), \sigma\}) \geq \max\{\Phi_+(b - \eta), \sigma\} \left[1 - B_{\lambda, \beta}(\max\{\Phi_+(b - \eta), \sigma\})\right] \end{aligned}$$

according to equation (2.10). Moreover, continuing the above chain of inequalities

$$\begin{aligned} \max\{a + \eta, \sigma\} &\geq \max\{\Phi_+(b - \eta), \Phi_+(\sigma)\} \left[1 - B_{\lambda, \beta}(\max\{a + \eta, \sigma\})\right] \\ &= \Phi_+(\max\{b - \eta, \sigma\}) \left[1 - B_{\lambda, \beta}(a + \eta)\right] \\ &\geq \max\{b - \eta, \sigma\} \frac{1 - B_{\lambda, \beta}(a + \eta)}{1 + B_{\lambda, \beta}(\max\{b - \eta, \sigma\})} \\ &\geq \max\{b - \eta, \sigma\} \frac{1 - B_{\lambda, \beta}(a + \eta)}{1 + B_{\lambda, \beta}(a + \eta)}. \end{aligned}$$

Therefore

$$\begin{aligned} \max\{b - \eta, \sigma\} &\leq \max\{a + \eta, \sigma\} \frac{1 + B_{\lambda, \beta}(a + \eta)}{1 - B_{\lambda, \beta}(a + \eta)} \\ &= \max\{a + \eta, \sigma\} \left(1 + \frac{2B_{\lambda, \beta}(a + \eta)}{1 - B_{\lambda, \beta}(a + \eta)}\right) \leq \max\{a + \eta, \sigma\} (1 + 2\tilde{B}_{\lambda, \beta}(a + \eta)) \end{aligned}$$

according to Lemma 5.5. This concludes the proof of **Step 1**.

Step 2 Taking the infimum in $(\lambda, \beta) \in \Lambda$ in equation (5.23), according to equation (5.13), we obtain that

$$\max\{b - \eta, \sigma\} \leq \max\{a + \eta, \sigma\} \left(1 + 2B_*(\min\{a + \eta, s_4^2\})\right).$$

We can then use the fact that $t \mapsto \max\{t, \sigma\} B_*(\min\{t, s_4^2\})$ is non-decreasing (proved in Lemma 5.7) to deduce that

$$\max\{b - \eta, \sigma\} \leq \max\{a + \eta, \sigma\} + 2 \max\{b + \eta, \sigma\} B_*(\min\{b + \sigma, s_4^2\}),$$

since there is nothing to prove when already $\max\{b + \eta, \sigma\} \leq \max\{a + \eta, \sigma\}$. Remark that $\max\{a + \eta, \sigma\} \leq \max\{a + \eta, \sigma + \eta\} \leq \max\{a, \sigma\} + \eta$ and that in the same way $\max\{b - \eta, \sigma\} \geq \max\{b, \sigma\} - \eta$. This proves that

$$\begin{aligned} \max\{b, \sigma\} - \max\{a, \sigma\} &\leq 2 \max\{a + \eta, \sigma\} B_*(\min\{a + \eta, s_4^2\}) + 2\eta \\ \text{and } \max\{b, \sigma\} - \max\{a, \sigma\} &\leq 2 \max\{b + \eta, \sigma\} B_*(\min\{b + \eta, s_4^2\}) + 2\eta. \end{aligned}$$

By symmetry, we can then exchange a and b to prove the same bounds for $\max\{a, \sigma\} - \max\{b, \sigma\}$, and therefore also for the absolute value of this quantity, which ends the proof of the lemma. \square

As a consequence the following result holds.

Corollary 5.1. *For any $(a, b) \in \mathbb{R}^2$ such that, for any $(\lambda, \beta) \in \Lambda$,*

$$\Phi_- \circ \Phi_+(a - \eta) \leq b + \eta, \quad \text{and} \quad \Phi_- \circ \Phi_+(b - \eta) \leq a + \eta,$$

and any threshold $\sigma \in \mathbb{R}_+$ such that $8\zeta(\sigma) \leq \sqrt{n}$ and $\sigma \leq s_4^2$, we have

$$\begin{aligned} |\max\{a, \sigma\} - \max\{b, \sigma\}| &\leq 2 \max\{a, \sigma\} B_*(\min\{a, s_4^2\}) + 5\eta/2 \\ |\max\{a, \sigma\} - \max\{b, \sigma\}| &\leq 2 \max\{b, \sigma\} B_*(\min\{b, s_4^2\}) + 5\eta/2. \end{aligned}$$

Proof. This is a consequence of the previous lemma, of the fact that $B_*(\min\{t, s_4^2\}) \leq 1/4$, and of the fact that $\max\{a + \eta, \sigma\} \leq \max\{a, \sigma\} + \eta$. \square

Appendix A: The Classical Empirical Estimator

The main goal of section 2 is to estimate the Gram matrix $G = \mathbb{E}(XX^\top)$, where $X \in \mathbb{R}^d$ is a random vector of unknown law $P \in \mathcal{M}_+^1(\mathbb{R}^d)$, from an i.i.d. sample $X_1, \dots, X_n \in \mathbb{R}^d$ drawn according to P . We have constructed a robust estimator of the Gram matrix and in section 4 we have shown empirically its performance in the case of a Gaussian mixture distribution. In this section we show from a theoretical point of view that the classical empirical estimator

$$\bar{G} = \frac{1}{n} \sum_{i=1}^n X_i X_i^\top$$

behaves similarly to our robust estimator in light tail situations, while it may perform worse otherwise.

As already done in section 2, we consider the quadratic form

$$N(\theta) = \theta^\top G \theta = \mathbb{E}(\langle \theta, X \rangle^2)$$

and we denote by

$$\bar{N}(\theta) = \theta^\top \bar{G} \theta = \frac{1}{n} \sum_{i=1}^n \langle \theta, X_i \rangle^2$$

the quadratic form associated to the empirical Gram matrix \bar{G} . According to the notation introduced in section 2, let $a > 0$ and let

$$K = 1 + \left\lceil a^{-1} \log \left(\frac{n}{72(2+c)\kappa^{1/2}} \right) \right\rceil$$

where $\kappa = \sup_{\substack{\theta \in \mathbb{R}^d \\ \mathbb{E}(\langle \theta, X \rangle^2) > 0}} \frac{\mathbb{E}(\langle \theta, X \rangle^4)}{\mathbb{E}(\langle \theta, X \rangle^2)^2}$ and $c = \frac{15}{8 \log(2)(\sqrt{2}-1)} \exp\left(\frac{1+2\sqrt{2}}{2}\right)$.

Let us put

$$R = \max_{i=1, \dots, n} \|X_i\| \quad (\text{A.1})$$

and let us introduce

$$\tau_*(t) = \frac{\lambda_*(t)^2 \exp(a/2) R^4}{3 \max\{t, \sigma\}^2}, \quad t \in \mathbb{R}_+,$$

where λ_* is defined in equation (5.15) as

$$\lambda_*(t) = \sqrt{\frac{2}{n(\kappa-1)} \left(\frac{(2+3c)\mathbb{E}(\|X\|^4)^{1/2}}{4(2+c)k^{1/2} \max\{t, \sigma\}} + \log(K/\epsilon) \right)}.$$

At the end of the section we mention some assumptions under which it is possible to give a non-random bound for R .

The following proposition, compared with the result obtained for the robust estimator $\hat{N}(\theta)$, presented in Proposition 2.3, shows that the different behavior of the two estimators \hat{N} and \bar{N} can appear only for heavy tail data distributions.

Proposition A.1. Consider any threshold $\sigma \in \mathbb{R}_+$ such that $\sigma \leq \mathbb{E}(\|X\|^4)^{1/2}$. With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$,

$$\left| \frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} - 1 \right| \leq B_*(N(\theta)) + \frac{\tau_*(N(\theta))}{[1 - \tau_*(N(\theta))]_+ [1 - B_*(N(\theta))]_+}.$$

where B_* is defined in Proposition 2.3.

Before proving the above proposition we observe that, also in this case, the bound does not depend explicitly on the dimension d of the ambient space and thus the result can be extended to any infinite-dimensional Hilbert space.

Proof. Let $\Lambda \subset (\mathbb{R}_+ \setminus \{0\})^2$ be the finite set defined in equation (2.11). We use as a tool the family of estimators

$$\tilde{N}_\lambda(\theta) = \frac{\lambda}{\hat{\alpha}(\theta)^2}$$

introduced in equation (2.4), where $\hat{\alpha}(\theta)$ is defined in equation (2.3). Let us put

$$\tau_\lambda(t) = \frac{\lambda^2 R^4}{3 \max\{t, \sigma\}^2}, \quad t \in \mathbb{R}_+.$$

We divide the proof into 4 steps.

Step 1. The first step consists in linking the empirical estimator \bar{N} with \tilde{N}_λ .

We claim that, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$, such that $\Phi_+(N(\theta)) > 0$,

$$\frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}} \leq \left[1 - \tau_\lambda(\tilde{N}_\lambda(\theta))\right]_+^{-1},$$

with the convention that $\frac{1}{0} = +\infty$. Moreover, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$, such that $\Phi_+(N(\theta)) > 0$,

$$\frac{\bar{N}(\theta)}{\tilde{N}_\lambda(\theta)} \geq 1 - \frac{\lambda^2}{3}.$$

We first observe that, according to the definition of $\hat{\alpha}(\theta)$, for any threshold $\sigma \in \mathbb{R}_+$,

$$\frac{1}{n} \sum_{i=1}^n \psi \left[\lambda \left(\max\{\tilde{N}_\lambda(\theta), \sigma\}^{-1} \langle \theta, X_i \rangle^2 - 1 \right) \right] \leq r \left(\lambda^{1/2} \tilde{N}_\lambda(\theta)^{-1/2} \theta \right) = r_\lambda \left(\hat{\alpha}(\theta) \theta \right) \leq 0,$$

where we have used the fact that the function ψ , introduced in equation (2.2), is non-decreasing. Moreover

$$r_\lambda \left(\hat{\alpha}(\theta) \theta \right) = 0$$

as soon as $\hat{\alpha}(\theta) < +\infty$ and this holds true, according to Proposition 2.1, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$ and any $(\lambda, \beta) \in \Lambda$ such that $\Phi_+(N(\theta)) > 0$. Indeed, by Proposition 2.1, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$,

$$\tilde{N}_\lambda(\theta) \geq \Phi_+(N(\theta)).$$

Defining $g(z) = z - \psi(z)$, we get

$$\begin{aligned} \frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}} - 1 &= \frac{1}{n\lambda} \sum_{i=1}^n \lambda \left(\langle \theta, X_i \rangle^2 \max\{\tilde{N}_\lambda(\theta), \sigma\}^{-1} - 1 \right) \\ &\leq \frac{1}{n\lambda} \sum_{i=1}^n g \left[\lambda \left(\langle \theta, X_i \rangle^2 \max\{\tilde{N}_\lambda(\theta), \sigma\}^{-1} - 1 \right) \right]. \end{aligned} \quad (\text{A.2})$$

In the same way, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$ such that $\Phi_+(N(\theta)) > 0$, we obtain

$$1 - \frac{\bar{N}(\theta)}{\tilde{N}_\lambda(\theta)} \leq \frac{1}{n\lambda} \sum_{i=1}^n g \left[\lambda \left(1 - \langle \theta, X_i \rangle^2 \tilde{N}_\lambda(\theta)^{-1} \right) \right]. \quad (\text{A.3})$$

We remark that the derivative of g is

$$g'(z) = 1 - \psi'(z) = \begin{cases} 1 & \text{if } z \notin [-1, 1] \\ \frac{\frac{z^2}{2}}{1 + z + \frac{z^2}{2}} & \text{if } z \in [-1, 0] \\ \frac{\frac{z^2}{2}}{1 - z + \frac{z^2}{2}} & \text{if } z \in [0, 1], \end{cases}$$

showing that $0 \leq g'(z) \leq z^2$, and therefore that g is a non-decreasing function satisfying

$$g(z) \leq \frac{1}{3} z_+^3. \quad (\text{A.4})$$

Applying equation (A.4) to equation (A.2) we obtain

$$\begin{aligned} \frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}} - 1 &\leq \frac{\lambda^2}{3n} \sum_{i=1}^n \left(\langle \theta, X_i \rangle^2 \max\{\tilde{N}_\lambda(\theta), \sigma\}^{-1} - 1 \right)_+^3 \\ &\leq \frac{\lambda^2}{3n \max\{\tilde{N}_\lambda(\theta), \sigma\}^3} \sum_{i=1}^n \langle \theta, X_i \rangle^6, \end{aligned}$$

where we have used the fact that $(z^2 - 1)_+ \leq z^2$. Since, by the Cauchy-Schwarz inequality, $\langle \theta, X_i \rangle^2 \leq \|\theta\|^2 R^2 = R^2$, we get

$$\begin{aligned} \frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}} - 1 &\leq \frac{\lambda^2}{3n \max\{\tilde{N}_\lambda(\theta), \sigma\}^3} R^4 \sum_{i=1}^n \langle \theta, X_i \rangle^2 \\ &= \frac{\lambda^2}{3} \times \frac{R^4}{\max\{\tilde{N}_\lambda(\theta), \sigma\}^2} \times \frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}}, \end{aligned}$$

which proves the first inequality. Similarly, since g is non-decreasing, we obtain that, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$ such that $\Phi_+(N(\theta)) > 0$,

$$1 - \frac{\bar{N}(\theta)}{\tilde{N}_\lambda(\theta)} \leq \frac{1}{n\lambda} \sum_{i=1}^n g(\lambda) \leq \frac{\lambda^2}{3},$$

where the last inequality follows from equation (A.4).

Step 2. This is an intermediate step. We claim that, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$, any $\sigma > 0$,

$$\begin{aligned} \max\{\bar{N}(\theta), \sigma\} &\leq \Phi_-^{-1}\left(\max\{N(\theta), \sigma\}\right) \left[1 - \tau_\lambda(N(\theta))\right]_+^{-1} \\ \max\{\bar{N}(\theta), \sigma\} &\leq \Phi_-^{-1}\left(\max\{N(\theta), \sigma\}\right) \left[1 - \tau_\lambda\left(\bar{N}(\theta)[1 - \tau_\lambda(\sigma)]_+\right)\right]_+^{-1} \\ \bar{N}(\theta) &\geq \left(1 - \frac{\lambda^2}{3}\right)_+ \Phi_+(N(\theta)) \end{aligned}$$

where Φ_+ and Φ_- are defined in Proposition 2.1.

We consider the threshold

$$\sigma' = \Phi_-^{-1}(\max\{N(\theta), \sigma\}) \geq \max\{N(\theta), \sigma\},$$

where we have used the fact that, by definition, $\Phi_-(t)^{-1} \geq t$, for any $t \in \mathbb{R}_+$. We assume that we are in the intersection of the two events of Proposition 2.1, which holds true with probability at least $1 - 2\epsilon$, so that

$$\sigma' \geq \max\{N(\theta), \sigma, \tilde{N}_\lambda(\theta)\}. \quad (\text{A.5})$$

According to **Step 1**, choosing as a threshold $\max\{\sigma, \sigma'\}$, we get

$$\frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma, \sigma'\}} \leq \left[1 - \tau_\lambda(\max\{\tilde{N}_\lambda(\theta), \sigma'\})\right]_+^{-1},$$

(where τ_λ is still defined with respect to σ), so that, according to equation (A.5),

$$\bar{N}(\theta) \leq \sigma' \left[1 - \tau_\lambda(\sigma')\right]_+^{-1}. \quad (\text{A.6})$$

As a consequence, recalling the definition of σ' , we have

$$\bar{N}(\theta) \leq \Phi_-^{-1}\left(\max\{N(\theta), \sigma\}\right) \left[1 - \tau_\lambda(N(\theta))\right]_+^{-1}.$$

Thus, observing that

$$\sigma \leq \Phi_-^{-1}(\sigma) \leq \Phi_-^{-1}\left(\max\{N(\theta), \sigma\}\right) \left[1 - \tau_\lambda(N(\theta))\right]_+^{-1},$$

we obtain the first inequality. To prove the second inequality, we use equation (A.6) once to see that

$$\sigma' \geq \bar{N}(\theta)[1 - \tau_\lambda(\sigma')]_+ \geq \bar{N}(\theta)[1 - \tau_\lambda(\sigma)]_+,$$

and we use it again to get

$$\begin{aligned} \bar{N}(\theta) &\leq \Phi_-^{-1}(\max\{N(\theta), \sigma\}) \left[1 - \tau_\lambda(\sigma')\right]_+^{-1} \\ &\leq \Phi_-^{-1}(\max\{N(\theta), \sigma\}) \left[1 - \tau_\lambda\left(\bar{N}(\theta)[1 - \tau_\lambda(\sigma)]_+\right)\right]_+^{-1}. \end{aligned}$$

To complete the proof of the second inequality, it is enough to remark that

$$\sigma \leq \Phi_-^{-1}(\sigma) \leq \Phi_-^{-1}\left(\max\{N(\theta), \sigma\}\right) \left[1 - \tau_\lambda\left(\bar{N}(\theta)[1 - \tau_\lambda(\sigma)]_+\right)\right]_+^{-1}.$$

To prove the last inequality, it is sufficient to remark that $\tilde{N}_\lambda(\theta) \geq \Phi_+(N(\theta))$ by Proposition 2.1 and hence, when $\Phi_+(N(\theta)) > 0$,

$$\bar{N}(\theta) \geq \left(1 - \frac{\lambda^2}{3}\right)_+ \Phi_+(N(\theta)).$$

On the other hand, when $\Phi_+(N(\theta)) = 0$, this inequality is also obviously satisfied.

Step 3. We now prove that, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$, any $\sigma > 0$,

$$\begin{aligned} \frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} - 1 &\leq \tilde{B}_{\lambda, \beta}(N(\theta)) + \frac{\tau_\lambda(N(\theta))}{[1 - \tau_\lambda(N(\theta))]_+ [1 - B_{\lambda, \beta}(N(\theta))]_+}, \\ 1 - \frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} &\leq B_{\lambda, \beta}(N(\theta)) + \frac{\lambda^2}{3}, \end{aligned}$$

where $B_{\lambda, \beta}$ is defined in equation (2.8) and $\tilde{B}_{\lambda, \beta}$ in equation (5.11).

We observe that, according to **Step 2**,

$$\begin{aligned} \max\{\bar{N}(\theta), \sigma\} &\leq \Phi_-^{-1}(\max\{N(\theta), \sigma\}) [1 - \tau_\lambda(N(\theta))]_+^{-1} \\ &\leq \frac{\max\{N(\theta), \sigma\}}{[1 - \tau_\lambda(N(\theta))]_+ [1 - B_{\lambda, \beta}(N(\theta))]_+}, \end{aligned}$$

which implies

$$\frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} - 1 \leq \frac{B_{\lambda, \beta}(N(\theta))}{[1 - B_{\lambda, \beta}(N(\theta))]_+} + \frac{\tau_\lambda(N(\theta))}{[1 - \tau_\lambda(N(\theta))]_+ [1 - B_{\lambda, \beta}(N(\theta))]_+}.$$

Applying Lemma 5.5 we obtain the first inequality.

To prove the second inequality we observe that, using again **Step 2**,

$$\begin{aligned}\max\{\bar{N}(\theta), \sigma\} &\geq \left(1 - \frac{\lambda^2}{3}\right)_+ \Phi_+(\max\{N(\theta), \sigma\}) \\ &= \left(1 - \frac{\lambda^2}{3}\right)_+ \max\{N(\theta), \sigma\} [1 + B_{\lambda, \beta}(N(\theta))]^{-1},\end{aligned}$$

where we have used the fact that $\Phi_+(\max\{z, \sigma\}) = \max\{z, \sigma\} (1 + B_{\lambda, \beta}(z))^{-1}$ as shown in equation (2.9). Thus we conclude that

$$1 - \frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} \leq \frac{B_{\lambda, \beta}(N(\theta)) + \lambda^2/3}{1 + B_{\lambda, \beta}(N(\theta))} \leq B_{\lambda, \beta}(N(\theta)) + \frac{\lambda^2}{3}.$$

Step 4. From **Step 3** we deduce that

$$\left| \frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} - 1 \right| \leq \tilde{B}_{\lambda, \beta}(N(\theta)) + \frac{\tau_\lambda(N(\theta))}{[1 - \tau_\lambda(N(\theta))]_+ [1 - B_{\lambda, \beta}(N(\theta))]_+}.$$

To conclude the proof it is sufficient to apply **Step 3** to $(\lambda_{\hat{\mathcal{J}}}, \beta_{\hat{\mathcal{J}}}) \in \Lambda$ defined in equation (2.11). Indeed, by equation (5.13), for any $t \in \mathbb{R}_+$,

$$B_{\lambda_{\hat{\mathcal{J}}}, \beta_{\hat{\mathcal{J}}}}(t) \leq B_*(t)$$

and, by equation (5.18), we have $\lambda_{\hat{\mathcal{J}}} \leq \lambda_*(\theta) \exp(a/4)$. \square

A.1. Non-random bounds for R

We conclude this section by mentioning assumptions under which it is possible to give a non-random bound for R , defined in equation (A.1).

Let us assume that, for some exponent $p \geq 1$ and some positive constants α and η ,

$$\mathbb{E} \left[\exp \left(\frac{\alpha}{2} \left(\frac{\|X\|^{2/p}}{\mathbf{Tr}(G)^{1/p}} - 1 - \eta^{2/p} \right) \right) \right] \leq 1.$$

In this case, with probability at least $1 - \epsilon$,

$$R \leq \mathbf{Tr}(G)^{1/2} \left(1 + \eta^{2/p} + 2\alpha^{-1} \log(n/\epsilon) \right)^{p/2}, \quad (\text{A.7})$$

where we recall that $\mathbf{Tr}(G) = \mathbb{E}[\|X\|^2]$.

To give a point of comparison, in the centered Gaussian case where $X \sim \mathcal{N}(0, G)$ is a Gaussian vector, we have, for any $\alpha \in [0, \lambda_1^{-1} \mathbf{Tr}(G)[$,

$$\mathbb{E} \left[\exp \left[\frac{\alpha}{2} \left(\frac{\|X\|^2}{\mathbf{Tr}(G)} + \frac{1}{\alpha} \sum_{i=1}^d \log \left(1 - \frac{\alpha \lambda_i}{\mathbf{Tr}(G)} \right) \right) \right] \right] = 1,$$

where $\lambda_1 \geq \dots \geq \lambda_d$ are the eigenvalues of G . Therefore, with probability at least $1 - \epsilon$,

$$R \leq \text{Tr}(G)^{1/2} \left(-\frac{1}{\alpha} \sum_{i=1}^d \log \left(1 - \frac{\alpha \lambda_i}{\text{Tr}(G)} \right) + \frac{2 \log(n/\epsilon)}{\alpha} \right)^{1/2}.$$

Moreover we observe that

$$\lim_{\alpha \rightarrow 0_+} -\frac{1}{\alpha} \sum_{i=1}^d \log \left(1 - \frac{\alpha \lambda_i}{\text{Tr}(G)} \right) = 1.$$

In order to replace equation (A.7) with some polynomial assumptions we need to replace R by

$$\tilde{R} = \left(\frac{1}{n} \sum_{i=1}^n \|X_i\|^6 \right)^{1/6}.$$

Indeed, by the Bienaymé Chebyshev inequality, we get that, with probability at least $1 - \epsilon$,

$$\tilde{R} \leq \left(\mathbb{E}[\|X\|^6] + \left(\frac{\mathbb{E}[\|X\|^{12}]}{n\epsilon} \right)^{1/2} \right)^{1/6} \leq \left(1 + (n\epsilon)^{-1/2} \right)^{1/6} \mathbb{E}[\|X\|^{12}]^{1/12}$$

and hence, with probability at least $1 - n^{-1}$,

$$\tilde{R} \leq 2^{1/6} \mathbb{E}[\|X\|^{12}]^{1/12}.$$

Also in the case where we consider this new quantity \tilde{R} we obtain a bound of the form of Proposition A.1. More precisely, the following proposition holds true.

Proposition A.2. *Let $0 < \sigma \leq \mathbb{E}(\|X\|^4)^{1/2}$ and let us put*

$$\zeta_*(t) = \frac{\lambda_*(t)^2 \exp(a/2) \tilde{R}^6}{3 \max\{t, \sigma\}^3}, \quad t \in \mathbb{R}_+.$$

With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$,

$$\left| \frac{\max\{\tilde{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} - 1 \right| \leq B_*(N(\theta)) + \frac{\zeta_*(N(\theta))}{[1 - B_*(N(\theta))]_+}.$$

Proof. We observe that another way to take advantage of equation (A.2) is to write

$$\frac{\tilde{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}} - 1 \leq \frac{\lambda^2 \|\theta\|^6}{3 \max\{\tilde{N}_\lambda(\theta), \sigma\}^3} \frac{1}{n} \sum_{i=1}^n \|X_i\|^6.$$

Thus, putting

$$\zeta_\lambda(t) = \frac{\lambda^2 \tilde{R}^6}{3 \max\{t, \sigma\}^3}, \quad t \in \mathbb{R}_+,$$

we get that, for any $\theta \in \mathbb{S}_d$,

$$\frac{\bar{N}(\theta)}{\max\{\tilde{N}_\lambda(\theta), \sigma\}} \leq 1 + \zeta_\lambda(\tilde{N}_\lambda(\theta)).$$

The same reasoning used to prove **Step 2** of Proposition [A.1](#) shows that, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$, any $\sigma > 0$,

$$\max\{\bar{N}(\theta), \sigma\} \leq \Phi^{-1}(\max\{N(\theta), \sigma\}) [1 + \zeta_\lambda(N(\theta))].$$

As a consequence, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$, any $(\lambda, \beta) \in \Lambda$,

$$\left| \frac{\max\{\bar{N}(\theta), \sigma\}}{\max\{N(\theta), \sigma\}} - 1 \right| \leq \tilde{B}_{\lambda, \beta}(N(\theta)) + \frac{\zeta_\lambda(N(\theta))}{[1 - B_{\lambda, \beta}(N(\theta))]_+}.$$

□

Appendix B: Generalization

In this section we come back to the finite-dimensional framework and we consider the problem of estimating the expectation of a symmetric random matrix. We will use these results to estimate the covariance matrix in the case of unknown expectation.

B.1. Symmetric random matrix

Let $A \in M_d(\mathbb{R})$ be a symmetric random matrix of size d . As already observed for the Gram matrix, the expectation of A can be recovered via the polarization identity from the quadratic form

$$N_A(\theta) = \mathbb{E} [\theta^\top A \theta], \quad \theta \in \mathbb{R}^d,$$

where the expectation is taken with respect to the unknown probability distribution of A on the space of symmetric matrices of size d . Observe that, if we decompose A in its positive and negative parts

$$A = A_+ - A_-,$$

the quadratic form N_A rewrites as

$$N_A(\theta) = \mathbb{E} [\theta^\top A_+ \theta] - \mathbb{E} [\theta^\top A_- \theta] = N_{A_+}(\theta) - N_{A_-}(\theta).$$

Thus in the following we will consider the case of a symmetric positive semi-definite random matrix of size d .

From now on let $A \in M_d(\mathbb{R})$ be a symmetric positive semi-definite random matrix of size d and let P be a probability distribution on the space of symmetric positive semi-definite random matrices of size d . Our goal is to estimate

$$N(\theta) = \mathbb{E} [\theta^\top A \theta], \quad \theta \in \mathbb{R}^d,$$

from an i.i.d. sample $A_1, \dots, A_n \in M_d(\mathbb{R})$ of symmetric positive semi-definite matrices drawn according to P . We observe that the quadratic form $N(\theta)$ rewrites as

$$N(\theta) = \mathbb{E} [\|A^{1/2} \theta\|^2]$$

where $A^{1/2}$ denotes the square root of A .

The construction of the (robust) estimator $\hat{N}(\theta)$ follows the one already done in the case of the Gram matrix with the necessary adjustments. For any $\lambda > 0$ and for any $\theta \in \mathbb{R}^d$, we consider the empirical criterion

$$r_\lambda(\theta) = \frac{1}{n} \sum_{i=1}^n \psi \left(\|A_i^{1/2} \theta\|^2 - \lambda \right),$$

where the influence function ψ is defined as in equation (2.2), and we perturb the parameter θ with the Gaussian perturbation $\pi_\theta \sim \mathcal{N}(\theta, \beta^{-1}I)$ of mean θ and

covariance matrix $\beta^{-1}\mathbf{I}$, where $\beta > 0$ is a free real parameter. We consider the family of estimators

$$\tilde{N}(\theta) = \frac{\lambda}{\hat{\alpha}(\theta)^2}$$

where $\hat{\alpha}(\theta) = \sup\{\alpha \in \mathbb{R}_+ \mid r_\lambda(\alpha\theta) \leq 0\}$. Let us put

$$s_4 = \mathbb{E}[\|A\|_\infty^2]^{1/4} \quad \text{and} \quad \kappa = \sup_{\substack{\theta \in \mathbb{R}^d \\ \mathbb{E}[\|A^{1/2}\theta\|^2] > 0}} \frac{\mathbb{E}[\|A^{1/2}\theta\|^4]}{\mathbb{E}[\|A^{1/2}\theta\|^2]^2}. \quad (\text{B.1})$$

The finite set $\Lambda \subset (\mathbb{R}_+ \setminus \{0\})^2$ of possible values of the couple of parameters (λ, β) is defined as

$$\Lambda = \{(\lambda_j, \beta_j) \mid 0 \leq j < K\},$$

where

$$K = 1 + \left\lceil a^{-1} \log \left(\frac{n}{72(2+c)\kappa^{1/2}} \right) \right\rceil, \quad (\text{B.2})$$

with $a > 0$, and

$$\begin{aligned} \lambda_j &= \sqrt{\frac{2}{(\kappa-1)n} \left(\frac{(2+3c)\mathbb{E}(\text{Tr}(A^2))}{4(2+c)\kappa^{1/2}\mathbb{E}(\|A\|_\infty^2)} \exp(ja) + \log(K/\epsilon) \right)}, \\ \beta_j &= \sqrt{2(2+c)\kappa^{1/2}\mathbb{E}(\|A\|_\infty^2) \exp[-(j-1/2)a]}. \end{aligned}$$

We recall that c is defined in equation (2.7) as $c = \frac{15}{8 \log(2)(\sqrt{2}-1)} \exp\left(\frac{1+2\sqrt{2}}{2}\right)$.

According to equation (2.8), let

$$B_{\lambda,\beta}(t) = \begin{cases} \frac{\gamma + \lambda\delta/\max\{t, \sigma\}}{1 - \mu - \gamma - 2\lambda\delta/\max\{t, \sigma\}} & (\lambda, \beta, t) \in \Gamma \\ +\infty & \text{otherwise} \end{cases}$$

and put $(\hat{\lambda}, \hat{\beta}) = \arg \min_{(\lambda,\beta) \in \Lambda} B_{\lambda,\beta}[\|\theta\|^{-2}\tilde{N}_\lambda(\theta)]$. Define the estimator \hat{N} as

$$\hat{N}(\theta) = \tilde{N}_{\hat{\lambda}}(\theta). \quad (\text{B.3})$$

Proposition B.1. *Let $\sigma \in]0, s_4^2]$ be some energy level. With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$,*

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\hat{N}(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq B_*[\|\theta\|^{-2}N(\theta)],$$

where B_* is defined as

$$B_*(t) = \begin{cases} \frac{n^{-1/2}\zeta_*(\max\{t, \sigma\})}{1 - 4n^{-1/2}\zeta_*(\max\{t, \sigma\})} & [6 + (\kappa-1)^{-1}]\zeta_*(\max\{t, \sigma\}) \leq \sqrt{n} \\ +\infty & \text{otherwise} \end{cases}$$

and

$$\zeta_*(t) = \sqrt{2.032(\kappa - 1) \left(\frac{0.73 \mathbb{E}[\mathbf{Tr}(A^2)]}{\kappa^{1/2} \mathbb{E}[\|A\|_\infty^2]^{1/2} t} + \log(K) + \log(\epsilon^{-1}) \right)} + \sqrt{\frac{98.5 \kappa^{1/2} \mathbb{E}[\|A\|_\infty^2]^{1/2}}{t}}.$$

As already discuss at the end of Proposition 2.3, if $a = 1/2$ and $n \leq 10^{20}$, we can bound the logarithmic factor $\log(K)$ with the (small) constant 4.35.

Proof. To prove Proposition B.1 we use many results already proved in the case of the Gram matrix (with the necessary adjustments).

We first observe that, denoting by $W \in \mathbb{R}^d$ a gaussian random vector with mean $A^{1/2}\theta$ and covariance matrix $\beta^{-1}A$, we have

$$\begin{aligned} \mathbb{E} \left[\|A^{1/2}\theta'\|^2 d\pi_\theta(\theta') \right] &= \sum_{i=1}^d \mathbb{E}(\langle W, e_i \rangle^2) \\ &= \|A^{1/2}\theta\|^2 + \frac{\mathbf{Tr}(A)}{\beta} \end{aligned}$$

where $\{e_i\}_{i=1}^d$ is the canonical basis of \mathbb{R}^d (and $\langle W, e_i \rangle$ is a one-dimensional Gaussian random variable with mean $\langle A^{1/2}\theta, e_i \rangle$ and variance $\beta^{-1}e_i^\top A e_i$). Therefore the empirical criterion rewrites as

$$r_\lambda(\theta) = \frac{1}{n} \sum_{i=1}^n \psi \left[\int \left(\|A_i^{1/2}\theta'\|^2 - \frac{\mathbf{Tr}(A_i)}{\beta} - \lambda \right) d\pi_\theta(\theta') \right].$$

We now use Lemma 5.3 to pull the expectation outside the influence function ψ . We decompose A into $A = UDU^\top$, where $UU^\top = I$ and $D = \text{diag}(\lambda_1, \dots, \lambda_d)$ and we observe that $U^\top\theta'$ has the same distribution as $U^\top\theta + W$, where $W \sim \mathcal{N}(0, \beta^{-1}I)$ so that

$$\begin{aligned} \mathbf{Var}[\|A^{1/2}\theta'\|^2 d\pi_\theta(\theta')] &= \mathbf{Var} \left(\sum_{i=1}^d ((U^\top\theta)_i + W_i)^2 \lambda_i \right) \\ &= \sum_{i=1}^d \lambda_i^2 \mathbf{Var}[(U^\top\theta)_i + W_i]^2 = \sum_{i=1}^d \left(\frac{2}{\beta^2} + \frac{4}{\beta} (U^\top\theta)_i^2 \right) \lambda_i^2 \\ &= \frac{2}{\beta^2} \mathbf{Tr}(A^2) + \frac{4}{\beta} \|A\theta\|^2. \end{aligned}$$

As a consequence we get

$$\begin{aligned} r_\lambda(\theta) &\leq \frac{1}{n} \sum_{i=1}^n \left[\int \chi \left(\|A_i^{1/2}\theta'\|^2 - \frac{\mathbf{Tr}(A_i)}{\beta} - \lambda \right) d\pi_\theta(\theta') \right. \\ &\quad \left. + \min \left\{ \log(4), \frac{1}{2\beta} \|A_i\theta\|^2 + \frac{\mathbf{Tr}(A_i^2)}{4\beta^2} \right\} \right] \end{aligned}$$

where the function χ is defined in equation (5.1). We then apply equation (5.4) with $m = \|A\theta\|$, $a = \log(4)$, $b = 1/(2\beta)$ and $c = \text{Tr}(A^2)/(4\beta^2)$ to obtain

$$r_\lambda(\theta) \leq \frac{1}{n} \sum_{i=1}^n \left[\int \chi \left(\|A^{1/2}\theta'\|^2 - \frac{\text{Tr}(A)}{\beta} - \lambda \right) d\pi_\theta(\theta') \right. \\ \left. + \int \min \left\{ 4\log(2), \frac{1}{\beta} \|A\theta'\|^2 + \frac{\text{Tr}(A^2)}{2\beta^2} \right\} d\pi_\theta(\theta') \right]$$

and we conclude, by Lemma 5.4, that

$$r_\lambda(\theta) \leq \frac{1}{n} \sum_{i=1}^n \int \log \left[1 + \|A_i^{1/2}\theta'\|^2 - \frac{\text{Tr}(A_i)}{\beta} - \lambda + \frac{1}{2} \left(\|A_i^{1/2}\theta'\|^2 - \frac{\text{Tr}(A_i)}{\beta} - \lambda \right)^2 \right. \\ \left. + \frac{c}{\beta} \left(\|A_i\theta'\|^2 + \frac{\text{Tr}(A_i^2)}{2\beta} \right) \right] d\pi_\theta(\theta'),$$

where $c = \frac{15}{8\log(2)(\sqrt{2}-1)} \exp\left(\frac{1+2\sqrt{2}}{2}\right)$. We then apply the PAC-Bayesian inequality (Proposition 5.1) to

$$f(A_i, \theta') = \log \left[1 + t(A_i, \theta') + \frac{1}{2} t(A_i, \theta')^2 + \frac{c}{\beta} \left(\|A_i\theta'\|^2 + \frac{\text{Tr}(A_i^2)}{2\beta} \right) \right]$$

where $t(A, \theta') = \|A^{1/2}\theta'\|^2 - \frac{\text{Tr}(A)}{\beta} - \lambda$ and we choose as posterior distributions the family of Gaussian perturbations π_θ . We obtain that, with probability at least $1 - \epsilon$, for any $\theta \in \mathbb{R}^d$,

$$r_\lambda(\theta) \leq \int \mathbb{E} \left[t(A, \theta') + \frac{1}{2} t(A, \theta')^2 + \frac{c}{\beta} \left(\|A\theta'\|^2 + \frac{\text{Tr}(A^2)}{2\beta} \right) \right] d\pi_\theta(\theta') \\ + \frac{\beta\|\theta\|^2}{2n} + \frac{\log(\epsilon^{-1})}{n} \\ = \mathbb{E} \left[\|A^{1/2}\theta\|^2 - \lambda + \frac{1}{2} \left(\|A^{1/2}\theta\|^2 - \lambda \right)^2 + \frac{(c+2)\|A\theta\|^2}{\beta} + \frac{(2+3c)\text{Tr}(A^2)}{2\beta^2} \right] \\ + \frac{\beta\|\theta\|^2}{2n} + \frac{\log(\epsilon^{-1})}{n}.$$

Using the Cauchy-Schwarz inequality remark that

$$\mathbb{E}[\|A\theta\|^2] \leq \mathbb{E}[\|A\|_\infty \|A^{1/2}\theta\|^2] \leq \mathbb{E}[\|A\|_\infty^2]^{1/2} \mathbb{E}[\|A^{1/2}\theta\|^4]^{1/2} \leq \mathbb{E}[\|A\|_\infty^2]^{1/2} \kappa^{1/2} N(\theta)$$

where κ is defined in equation (B.1). Thus

$$\begin{aligned} r_\lambda(\theta) &\leq \frac{\kappa}{2} [N(\theta) - \lambda]^2 + \left[1 + (\kappa - 1)\lambda + \frac{(2+c)\kappa^{1/2}\mathbb{E}[\|A\|_\infty^2]^{1/2}}{\beta} \right] [N(\theta) - \lambda] \\ &+ \frac{(\kappa - 1)\lambda^2}{2} + \frac{(2+c)\kappa^{1/2}\mathbb{E}[\|A\|_\infty^2]^{1/2}\lambda}{\beta} + \frac{(2+3c)\mathbb{E}[\text{Tr}(A^2)]}{2\beta^2} + \frac{\beta\|\theta\|^2}{2n} + \frac{\log(\epsilon^{-1})}{n}. \end{aligned}$$

This is the analogous of equation (5.5). Thus, proceeding as already done in the case of the Gram matrix we conclude the proof. \square

Remark that to obtain the above result we have used the fact that

$$\mathbb{E}[\|A\theta\|^2] \leq \mathbb{E}[\|A\|_\infty^2]^{1/2} \kappa^{1/2} N(\theta).$$

However, if we use any upper bound of the form

$$\mathbb{E}[\|A\theta\|^2] \leq f(\mathbb{E}[A])N(\theta)$$

Proposition B.1 holds replacing $\mathbb{E}[\|A\|_\infty^2]^{1/2} \kappa^{1/2}$ with $f(\mathbb{E}[A])$ in the definition of ζ_* . Similarly we can replace $\mathbb{E}[\text{Tr}(A^2)]$ by an upper bound.

We observe in particular that

$$\frac{\mathbb{E}[\|A\|_\infty^2]^{1/2}}{\kappa^{1/2}} \leq \frac{\mathbb{E}[\text{Tr}(A^2)]}{\kappa^{1/2}\mathbb{E}[\|A\|_\infty^2]^{1/2}} \leq \mathbb{E}[\text{Tr}(A)] = \text{Tr}[\mathbb{E}(A)].$$

Indeed, to see the first inequality it is sufficient to observe that $\|A\|_\infty^2 \leq \text{Tr}(A^2)$. Moreover we have that

$$\mathbb{E}[\text{Tr}(A^2)] \leq \mathbb{E}[\|A\|_\infty \text{Tr}(A)] \leq \mathbb{E}[\|A\|_\infty^2]^{1/2} \mathbb{E}[\text{Tr}(A)^2]^{1/2},$$

and, denoting by $\{e_i\}_{i=1}^d$ an orthonormal basis of \mathbb{R}^d ,

$$\begin{aligned} \mathbb{E}[\text{Tr}(A)^2] &= \sum_{\substack{1 \leq i \leq d, \\ 1 \leq j \leq d}} \mathbb{E}[\|A^{1/2}e_i\|^2 \|A^{1/2}e_j\|^2] \\ &\leq \sum_{\substack{1 \leq i \leq d, \\ 1 \leq j \leq d}} \mathbb{E}[\|A^{1/2}e_i\|^4]^{1/2} \mathbb{E}[\|A^{1/2}e_j\|^4]^{1/2} \\ &\leq \kappa \sum_{\substack{1 \leq i \leq d, \\ 1 \leq j \leq d}} \mathbb{E}[\|A^{1/2}e_i\|^2] \mathbb{E}[\|A^{1/2}e_j\|^2] = \kappa \mathbb{E}[\text{Tr}(A)]^2. \end{aligned}$$

This implies that we can bound ζ_* in Proposition B.1 by

$$\zeta_*(t) = \sqrt{2.032(\kappa - 1) \left(\frac{0.73 \mathbb{E}[\text{Tr}(A)]}{t} + \log(K) + \log(\epsilon^{-1}) \right)} + \sqrt{\frac{98.5 \kappa \mathbb{E}[\text{Tr}(A)]}{t}}. \quad (\text{B.4})$$

We conclude this section observing that, since the entropy terms are dominated by $\mathbb{E}[\text{Tr}(A)]$, the result can be generalized to the case where A is a random symmetric positive semi-definite operator in a infinite-dimensional Hilbert space with the only additional assumption that $\mathbb{E}[\text{Tr}(A)] < +\infty$.

B.2. Covariance matrix

Let $X \in \mathbb{R}^d$ be a random vector distributed according to the unknown probability measure $P \in \mathcal{M}_+^1(\mathbb{R}^d)$. The covariance matrix of X is defined by

$$\Sigma = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^\top]$$

and our goal is to estimate, uniformly in θ , the quadratic form

$$N(\theta) = \theta^\top \Sigma \theta = \mathbb{E}[\langle \theta, X - \mathbb{E}[X] \rangle^2], \quad \theta \in \mathbb{R}^d,$$

from an i.i.d. sample $X_1, \dots, X_n \in \mathbb{R}^d$ drawn according to P . We cannot use the results we have proved for the Gram matrix, since the quadratic form N depends on the unknown quantity $\mathbb{E}[X]$. However we can find a workaround, using the results of the previous section about symmetric random matrices. Indeed, we do not need to estimate $\mathbb{E}[X]$ in order to estimate N but it is sufficient to observe that the quadratic form N can be written as

$$N(\theta) = \frac{1}{2} \mathbb{E}[\langle \theta, X - X' \rangle^2]$$

where X' is an independent copy of X . More generally, given $q \in \mathbb{N}$, we may consider q independent copies $X^{(1)}, \dots, X^{(q)}$ of X and the random matrix

$$A = \frac{1}{q(q-1)} \sum_{1 \leq j < k \leq q} (X^{(j)} - X^{(k)})(X^{(j)} - X^{(k)})^\top$$

so that

$$N(\theta) = \frac{1}{q(q-1)} \mathbb{E} \left[\sum_{1 \leq j < k \leq q} \langle \theta, X^{(j)} - X^{(k)} \rangle^2 \right] = \mathbb{E}[\theta^\top A \theta].$$

We will discuss later how to choose q . In the following we use a robust block estimate which consists in dividing the sample X_1, \dots, X_n in blocks of size q and then in considering the original sample as a "new" sample of $\lfloor n/q \rfloor$ symmetric matrices $A_1, \dots, A_{\lfloor n/q \rfloor}$ (of independent copies of A) defined as

$$A_i = \frac{1}{q(q-1)} \sum_{(i-1)q < j < k \leq iq} (X_j - X_k)(X_j - X_k)^\top$$

that thus correspond to the empirical covariance estimates on each block. We can use the results of the previous section to define a robust estimator of $N(\theta)$.

Let us introduce

$$\kappa' = \sup_{\substack{\theta \in \mathbb{R}^d, \\ \mathbb{E}(\|A^{1/2}\theta\|^2) > 0}} \frac{\mathbb{E}[\|A^{1/2}\theta\|^4]}{\mathbb{E}[\|A^{1/2}\theta\|^2]^2},$$

$$\text{and } \kappa = \sup_{\substack{\theta \in \mathbb{R}^d, \\ \mathbb{E}[\langle \theta, X - \mathbb{E}(X) \rangle^2] > 0}} \frac{\mathbb{E}[\langle \theta, X - \mathbb{E}(X) \rangle^4]}{\mathbb{E}[\langle \theta, X - \mathbb{E}(X) \rangle^2]^2}.$$

Lemma B.1. *The two kurtosis coefficients introduced above are related by the relation*

$$\kappa' \leq 1 + \tau_q(\kappa)/q,$$

$$\text{where } \tau_q(\kappa) = \kappa - 1 + \frac{2}{q-1}.$$

Proof. Replacing X with $X - \mathbb{E}[X]$ we may assume during the proof that $\mathbb{E}[X] = 0$. It holds that

$$\begin{aligned} \mathbb{E}[\|A^{1/2}\theta\|^4] &= \mathbb{E}\left[\left(\frac{1}{q(q-1)} \sum_{1 \leq j < k \leq q} \langle \theta, X^{(j)} - X^{(k)} \rangle^2\right)^2\right] \\ &= \frac{1}{q^2(q-1)^2} \sum_{\substack{1 \leq j < k \leq q \\ 1 \leq s < t \leq q}} \mathbb{E}[\langle \theta, X^{(j)} - X^{(k)} \rangle^2 \langle \theta, X^{(s)} - X^{(t)} \rangle^2] \end{aligned}$$

Recalling the definition of covariance, we have

$$\begin{aligned} \mathbb{E}[\|A^{1/2}\theta\|^4] &= \frac{1}{q^2(q-1)^2} \left\{ \sum_{\substack{1 \leq j < k \leq q \\ 1 \leq s < t \leq q}} \mathbb{E}[\langle \theta, X^{(j)} - X^{(k)} \rangle^2] \mathbb{E}[\langle \theta, X^{(s)} - X^{(t)} \rangle^2] \right. \\ &\quad + \sum_{1 \leq j < k \leq q} \mathbb{E}[\langle \theta, X^{(j)} - X^{(k)} \rangle^4] - \mathbb{E}[\langle \theta, X^{(j)} - X^{(k)} \rangle^2]^2 \\ &\quad + \sum_{\substack{1 \leq j < k \leq q \\ 1 \leq s < t \leq q \\ |\{j,k\} \cap \{s,t\}| = 1}} \left(\mathbb{E}[\langle \theta, X^{(j)} - X^{(k)} \rangle^2 \langle \theta, X^{(s)} - X^{(t)} \rangle^2] \right. \\ &\quad \left. \left. - \mathbb{E}[\langle \theta, X^{(j)} - X^{(k)} \rangle^2] \mathbb{E}[\langle \theta, X^{(s)} - X^{(t)} \rangle^2] \right) \right\} \\ &= \frac{1}{4} \mathbb{E}[\langle \theta, X^{(2)} - X^{(1)} \rangle^2]^2 + \frac{1}{2q(q-1)} \mathbb{E}[\langle \theta, X^{(2)} - X^{(1)} \rangle^4] - \mathbb{E}[\langle \theta, X^{(2)} - X^{(1)} \rangle^2]^2 \\ &\quad + \frac{q-2}{q(q-1)} \left(\mathbb{E}[\langle \theta, X^{(1)} - X^{(2)} \rangle^2 \langle \theta, X^{(1)} - X^{(3)} \rangle^2] - \mathbb{E}[\langle \theta, X^{(1)} - X^{(2)} \rangle^2]^2 \right). \end{aligned}$$

Define $W_j = \langle \theta, X^{(j)} \rangle$ and observe that

$$\begin{aligned}\mathbb{E}[(W_1 - W_2)^2]^2 &= 4N(\theta)^2, \\ \mathbb{E}[(W_1 - W_2)^4] &= \mathbb{E}[W_1^4] + 6\mathbb{E}[W_1^2]\mathbb{E}[W_2^2] + \mathbb{E}[W_2^4] \\ &= 2\mathbb{E}[W_1^4] + 6\mathbb{E}[W_1^2]^2 \leq (2\kappa + 6)N(\theta)^2, \\ \mathbb{E}[(W_1 - W_2)^2(W_1 - W_3)^2] &= \mathbb{E}[W_1^4] + 3\mathbb{E}[W_2^2]^2 \leq (\kappa + 3)N(\theta)^2.\end{aligned}$$

Therefore

$$\mathbb{E}[\|A^{1/2}\theta\|^4] \leq \left(1 + \frac{(q-2)(\kappa-1)}{q(q-1)} + \frac{(\kappa+1)}{q(q-1)}\right)N(\theta)^2 = \left(1 + \frac{\tau_q(\kappa)}{q}\right)N(\theta)^2,$$

and hence $\kappa' \leq 1 + \tau_q(\kappa)/q$, since $\mathbb{E}[\|A^{1/2}\theta\|^2] = N(\theta)$. \square

Let $\widehat{N}(\theta)$ be the estimator defined in equation (B.3) and remark that

$$\mathbb{E}(\mathbf{Tr}(A)) = \mathbf{Tr}(\mathbb{E}(A)) = \mathbf{Tr}(\Sigma) = \mathbb{E}(\|X - \mathbb{E}(X)\|^2)$$

Proposition B.2. *For any energy level $\sigma \in]0, \mathbf{Tr}(\Sigma)]$, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{R}^d$,*

$$\left| \frac{\max\{N(\theta), \sigma\|\theta\|^2\}}{\max\{\widehat{N}(\theta), \sigma\|\theta\|^2\}} - 1 \right| \leq B_*\left(\|\theta\|^{-2}N(\theta)\right),$$

where

$$B_*(t) = \begin{cases} \frac{(q\lfloor n/q \rfloor)^{1/2}\zeta_q(\max\{t, \sigma\})}{1 - 4(q\lfloor n/q \rfloor)^{1/2}\zeta_q(\max\{t, \sigma\})}, & \text{if } (6 + q/\tau_q(\kappa))\zeta_q(\max\{t, \sigma\}) \leq (q\lfloor n/q \rfloor)^{1/2}, \\ +\infty, & \text{otherwise} \end{cases}$$

and

$$\zeta_q(t) = \sqrt{2.032\tau_q(\kappa)\left(\frac{0.73\mathbf{Tr}(\Sigma)}{t} + \log(K) + \log(\epsilon^{-1})\right)} + \sqrt{\frac{98.5(q + \tau_q(\kappa))\mathbf{Tr}(\Sigma)}{t}}$$

with K defined in equation (B.2).

Proof. The result follows from Proposition B.1, using the definition of ζ_* given in equation (B.4), where we replace κ by κ' and n by $\lfloor n/q \rfloor$. According to Lemma B.1 we conclude the proof. \square

Here we have used the upper bound for the entropy factor defined in terms of $\mathbb{E}[\mathbf{Tr}(A)] = \mathbf{Tr}(\Sigma)$, as mentioned in the remarks following Proposition B.1. We can improve somehow the constants by evaluating more carefully $\mathbb{E}[\|A\theta\|^2]$ and $\mathbb{E}[\mathbf{Tr}(A^2)]$.

Lemma B.2. *It holds that*

$$\mathbb{E}[\|A\theta\|^2] \leq \left(1 - \frac{q-2}{q(q-1)}\right) \|\Sigma\|_\infty N(\theta) + \frac{1}{q} \left(\kappa + \frac{1}{q-1}\right) \mathbf{Tr}(\Sigma) N(\theta) \quad (\text{B.5})$$

$$\mathbb{E}[\mathbf{Tr}(A^2)] \leq \left(1 - \frac{q-2}{q(q-1)}\right) \mathbf{Tr}(\Sigma^2) + \frac{1}{q} \left(\kappa + \frac{1}{q-1}\right) \mathbf{Tr}(\Sigma)^2. \quad (\text{B.6})$$

Proof. Replacing X with $X - \mathbb{E}[X]$ we may assume that $\mathbb{E}[X] = 0$. Recall that

$$\mathbb{E}[\|X\|^4] \leq \kappa \mathbb{E}[\|X\|^2]^2 = \kappa \mathbf{Tr}(\Sigma)^2$$

and $\mathbb{E}[\langle X^{(1)}, X^{(2)} \rangle^2] = \mathbf{Tr}(\Sigma^2)$. We observe that

$$\mathbb{E}[\|A\theta\|^2] = \mathbb{E} \left[\frac{1}{q^2(q-1)^2} \sum_{\substack{1 \leq j < k \leq q \\ 1 \leq s < t \leq q}} \langle \theta, X^{(j)} - X^{(k)} \rangle \langle X^{(j)} - X^{(k)}, X^{(s)} - X^{(t)} \rangle \langle X^{(s)} - X^{(t)}, \theta \rangle \right]$$

and

$$\begin{aligned} & \mathbb{E} \left[\langle \theta, X^{(1)} - X^{(2)} \rangle \langle X^{(1)} - X^{(2)}, X^{(3)} - X^{(4)} \rangle \langle X^{(3)} - X^{(4)}, \theta \rangle \right] \\ &= 4 \mathbb{E} \left[\langle \theta, X^{(1)} \rangle \langle X^{(1)}, X^{(2)} \rangle \langle X^{(2)}, \theta \rangle \right] = 4 \|\Sigma \theta\|^2 \leq 4 \|\Sigma\|_\infty N(\theta), \\ & \mathbb{E} \left[\langle \theta, X^{(1)} - X^{(2)} \rangle \langle X^{(1)} - X^{(2)}, X^{(1)} - X^{(3)} \rangle \langle X^{(1)} - X^{(3)}, \theta \rangle \right] \\ &= \mathbb{E} \left[\langle \theta, X^{(1)} \rangle^2 \|X^{(1)}\|^2 \right] + 3 \mathbb{E} \left[\langle \theta, X^{(1)} \rangle \langle X^{(1)}, X^{(2)} \rangle \langle X^{(2)}, \theta \rangle \right] \\ &\leq \kappa \mathbf{Tr}(\Sigma) N(\theta) + 3 \|\Sigma\|_\infty N(\theta), \\ & \mathbb{E} \left[\langle \theta, X^{(1)} - X^{(2)} \rangle \langle X^{(1)} - X^{(2)}, X^{(1)} - X^{(2)} \rangle \langle X^{(1)} - X^{(2)}, \theta \rangle \right] \\ &= 2 \mathbb{E} \left[\langle \theta, X^{(1)} \rangle^2 \|X^{(1)}\|^2 \right] + 2 \mathbb{E} \left[\langle \theta, X^{(1)} \rangle^2 \right] \mathbb{E} [\|X^{(1)}\|^2] \\ &\quad + 4 \mathbb{E} \left[\langle \theta, X^{(1)} \rangle \langle X^{(1)}, X^{(2)} \rangle \langle X^{(2)}, \theta \rangle \right] \\ &\leq 2(\kappa + 1) \mathbf{Tr}(\Sigma) N(\theta) + 4 \|\Sigma\|_\infty N(\theta), \end{aligned}$$

which proves the first inequality. In the same way,

$$\mathbb{E}[\mathbf{Tr}(A^2)] = \mathbb{E} \left[\frac{1}{q^2(q-1)^2} \sum_{\substack{1 \leq j < k \leq q \\ 1 \leq s < t \leq q}} \langle X^{(j)} - X^{(k)}, X^{(s)} - X^{(t)} \rangle^2 \right],$$

and

$$\begin{aligned}
\mathbb{E}\left[\langle X^{(1)} - X^{(2)}, X^{(3)} - X^{(4)} \rangle^2\right] &= 4\mathbb{E}\left[\langle X^{(1)}, X^{(2)} \rangle^2\right] \\
&= 4\mathbf{Tr}(\Sigma^2), \\
\mathbb{E}\left[\langle X^{(1)} - X^{(2)}, X^{(1)} - X^{(3)} \rangle^2\right] &= \mathbb{E}\left[\|X^{(1)}\|^4\right] + 3\mathbb{E}\left[\langle X^{(1)}, X^{(2)} \rangle^2\right] \\
&\leq \kappa\mathbf{Tr}(\Sigma)^2 + 3\mathbf{Tr}(\Sigma^2), \\
\mathbb{E}\left[\langle X^{(1)} - X^{(2)}, X^{(1)} - X^{(2)} \rangle^2\right] &= 2\mathbb{E}\left[\|X^{(1)}\|^4\right] + 2\mathbb{E}\left[\|X^{(1)}\|^2\right]^2 + 4\mathbb{E}\left[\langle X^{(1)}, X^{(2)} \rangle^2\right] \\
&\leq 2(\kappa + 1)\mathbf{Tr}(\Sigma)^2 + 4\mathbf{Tr}(\Sigma^2),
\end{aligned}$$

which concludes the proof. \square

Using these tighter bounds, we can improve ζ_q to

$$\begin{aligned}
\zeta_q(t) &= \left[2.032 \tau_q(\kappa) \left(\frac{0.73 \left[\left(1 - \frac{q-2}{q(q-1)}\right) \mathbf{Tr}(\Sigma^2) + \frac{1}{q} \left(\kappa + \frac{1}{q-1}\right) \mathbf{Tr}(\Sigma)^2 \right]}{\left[\left(1 - \frac{q-2}{q(q-1)}\right) \|\Sigma\|_\infty + \frac{1}{q} \left(\kappa + \frac{1}{q-1}\right) \mathbf{Tr}(\Sigma) \right] t} \right. \right. \\
&\quad \left. \left. + \log(K) + \log(\epsilon^{-1}) \right) \right]^{1/2} \\
&\quad + \sqrt{\frac{98.5 \left[q \left(1 - \frac{q-2}{q(q-1)}\right) \|\Sigma\|_\infty + \left(\kappa + \frac{1}{q-1}\right) \mathbf{Tr}(\Sigma) \right]}{t}}.
\end{aligned}$$

Therefore, in the case when

$$q\|\Sigma\|_\infty \leq \mathbf{Tr}(\Sigma),$$

we have

$$\mathbb{E}\left[\|A\theta\|^2\right] \leq \frac{1}{q} \left(\kappa + 1 + \frac{2}{q(q-1)} \right) \mathbf{Tr}(\Sigma) N(\theta)$$

and hence, recalling that $\mathbf{Tr}(\Sigma^2) \leq \mathbf{Tr}(\Sigma)^2$, we can take

$$\zeta_q(t) = \sqrt{2.032 \tau_q(\kappa) \left(\frac{0.73 \mathbf{Tr}(\Sigma)}{t} + \log(K) + \log(\epsilon^{-1}) \right)} + \sqrt{\frac{98.5 \left(\kappa + 1 + \frac{2}{q(q-1)} \right) \mathbf{Tr}(\Sigma)}{t}}.$$

If we compare the above result with the bound obtained in Proposition 2.3 for the Gram matrix estimator, we see that the first appearance of κ in the definition of ζ_q has been replaced with

$$\tau_q(\kappa) + 1 = \kappa + \frac{2}{q-1},$$

and that the second appearance of κ has been replaced with

$$\kappa + 1 + \frac{2}{q(q-1)}.$$

Thus, when $\|\Sigma\|_\infty \leq \text{Tr}(\Sigma)/2$, that is not a very strong hypothesis, we can take at least $q = 2$, and obtain an improved bound for the estimation of Σ that is not much larger than the bound for the estimation of the centered Gram matrix, that requires the knowledge of $\mathbb{E}(X)$, since the difference between the two bounds is just a matter of replacing κ with $\kappa + 2$.

References

- Catoni, O. (2012) *Challenging the empirical mean and empirical variance: a deviation study*. Ann. Inst. Henri Poincaré Probab. Stat. 48(4):1148–1185
- Catoni, O. (2015) *Estimating the gram matrix and least square regression through pac-bayes bounds*. preprint
- Giulini, I. (2015) *Generalization bounds for random samples in Hilbert spaces*. Ph.D. Thesis
- Koltchinskii, V. and Giné, E. (2000) *Random matrix approximation of spectra of integral operators*. Bernoulli 6(1):113–167
- Koltchinskii, V. and Lounici, K. (2014) *Asymptotics and concentration bounds for spectral projectors of sample covariance*. preprint [arXiv:1408.4643](https://arxiv.org/abs/1408.4643)
- Minsker, S. *Geometric median and robust estimation in banach spaces*. to appear
- Rosasco, L., Belkin, M. and De Vito, E. (2010) *On learning with integral operators*. Journal of Machine Learning Research, 11:905–934
- Rudelson, M. *Random vectors in the isotropic position*. J. Funct. Anal., 164(1):60–72
- Shawe-Taylor, J., Williams, C. and Cristianini, C. and Kandola, J. (2005) *On the eigenspectrum of the gram matrix and its relationship to the operator eigenspectrum*. Eds.): ALT 2002, LNAI 2533, pages 23–40, Springer-Verlag
- Shawe-Taylor, J., Williams, C. and Cristianini, C. and Kandola, J. (2005) *On the Eigenspectrum of the Gram Matrix and the Generalisation Error of Kernel PCA*. IEEE Transactions on Information Theory
- Tropp, J. A. (2012) *User-friendly tail bounds for sums of random matrices*. Found. Comput. Math., 12(4):389–434
- Vershynin, R. (2012) *Introduction to the non-asymptotic analysis of random matrices*. In Compressed sensing, pages 210–268. Cambridge Univ. Press, Cambridge
- von Luxburg, U., Belkin, M. and Bousquet, O. (2008) *Consistency of spectral clustering*. Ann. Statist., 36(2):555–586
- Zwald, L., Bousquet, O. and Blanchard, G. (2004) *Statistical properties of kernel principal component analysis*. In Learning theory, volume 3120 of Lecture Notes in Comput. Sci., pages 594–608. Springer, Berlin